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# Bis[chloridobis(triphenylphosphine)-copper(I)-$\mu$-chlorido]bis(1,2-diaminopropane)copper(II) acetonitrile disolvate

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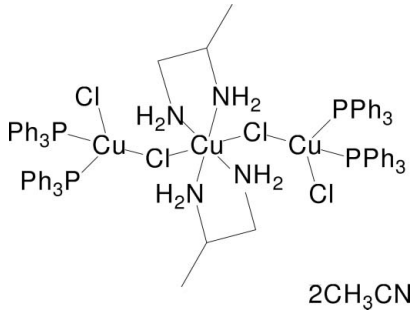
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.007 Å; disorder in main residue; $R$ factor = 0.054; $wR$ factor = 0.158; data-to-parameter ratio = 14.0.

The title complex [systematic name: bis(1,2-diaminopropane-2$\kappa^2N$,$N'$)di-$\mu$-chlorido-1:2$\kappa^2Cl$,2:3$\kappa^2Cl$-dichlorido-1$\kappa Cl$,3$\kappa Cl$-tetrakis(triphenylphosphine)-1$\kappa^2P$,3$\kappa^2P$-tricopper(I,II,I) acetonitrile disolvate], $[\{(Ph_3P)_2Cl_2Cu\}_2Cu(C_3H_{10}N_2)_2]\cdot 2C_2H_3N$, is a centrosymmetric linear trinuclear mixed-valence copper complex in which the central $Cu^{II}$ atom is bridged by Cl atoms to the two $Cu^{I}$ atoms. The coordination geometry is octahedral for $Cu^{II}$, with Jahn–Teller elongation of the Cu—Cl bonds, and distorted tetrahedral for $Cu^{I}$, with a wide P—Cu—P angle. The diamine ligands are twofold disordered, with occupancy factors of *ca* 0.6:0.4, and form one N—H···Cl hydrogen bond each with a terminal Cl atom.

## Related literature

For related structures, see: Arrizabalaga *et al.* (1983); Bailey *et al.* (1995); Choi *et al.* (2006); Feng *et al.* (2007); Onan *et al.* (1984); Prins *et al.* (1996).




## Experimental

### Crystal data

$[Cu_3Cl_4(C_3H_{10}N_2)_2(C_{18}H_{15}P)_4]\cdot 2C_2H_3N$
$M_r$ = 1611.87
Monoclinic, $P2_1/c$
$a$ = 15.896 (3) Å
$b$ = 9.4181 (15) Å
$c$ = 26.533 (4) Å
$\beta$ = 94.957 (12)°
$V$ = 3957.4 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.06 mm$^{-1}$
$T$ = 150 (2) K
0.25 × 0.20 × 0.20 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min}$ = 0.780, $T_{max}$ = 0.820
32758 measured reflections
6923 independent reflections
5038 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.074

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.158
$S$ = 1.03
6923 reflections
496 parameters
136 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.81 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—Cl1 | 2.3553 (13) | Cu2—N1 | 2.042 (10) |
| Cu1—Cl2 | 2.4372 (13) | Cu2—N2 | 1.995 (10) |
| Cu1—P1 | 2.2800 (13) | Cu2—N1*X* | 2.065 (14) |
| Cu1—P2 | 2.2835 (12) | Cu2—N2*X* | 1.995 (18) |
| Cu2—Cl2 | 2.8731 (12) | | |
| Cl1—Cu1—Cl2 | 101.06 (5) | Cl2—Cu2—N1 | 92.9 (3) |
| Cl1—Cu1—P1 | 111.76 (5) | Cl2—Cu2—N2 | 87.4 (3) |
| Cl1—Cu1—P2 | 105.75 (5) | Cl2—Cu2—N1*X* | 93.6 (4) |
| Cl2—Cu1—P1 | 108.31 (5) | Cl2—Cu2—N2*X* | 93.8 (5) |
| Cl2—Cu1—P2 | 105.94 (5) | N1—Cu2—N2 | 84.4 (4) |
| P1—Cu1—P2 | 121.92 (4) | N1*X*—Cu2—N2*X* | 84.7 (6) |
| Cu1—Cl2—Cu2 | 122.71 (5) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···Cl1$^{i}$ | 0.92 | 2.45 | 3.330 (9) | 159 |
| N2*X*—H2*X*1···Cl1$^{i}$ | 0.92 | 2.60 | 3.495 (15) | 163 |

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2455).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2305-m2306 [ **doi:10.1107/S1600536807037282** ]

# Bis[chloridobis(triphenylphosphine)copper(I)-$\mu$-chlorido]bis(1,2-diaminopropane)copper(II) acetonitrile disolvate

**M. H. Habibi, M. Mikhak, R. W. Harrington and W. Clegg**

## Comment

Trinuclear metal complexes can be classified as linear and non-linear. Trinuclear copper complexes with two, three or four bridges (Prins *et al*., 1996; Feng *et al.*, 2007; Onan *et al.*, 1984; Choi *et al*., 2006) have been reported. There are also some reported singly-bridged copper complexes (Arrizabalaga *et al.*, 1983; Bailey *et al.*, 1995). We report here the crystal structure of a new linear trinuclear mixed-valence copper compound, (I) (Fig. 1). It contains two $Cu^{I}$ atoms with distorted tetrahedral coordination, the four vertices being occupied by two P atoms of $PPh_3$ ligands and two Cl atoms. The largest deviation from ideal tetrahedral geometry is the wide P—Cu—P angle of 121.92 (4)°. The central $Cu^{II}$ atom lies on an inversion centre and has octahedral coordination, with two chelating bidentate diamines and two *trans*-chloro bridges to the $Cu^{I}$ atoms. The diamine ligands are disordered over two orientations, with refined occupancy factors of 0.599:0.401 (10). Each of them forms one N—H···Cl hydrogen bond to a terminal Cl atom. The Cu—Cl bonds for the central $Cu^{II}$ atom are elongated as a result of a typical Jahn-Teller distortion, and the bridging Cl atoms make longer bonds to the $Cu^{I}$ atoms than do the terminal Cl atoms, as expected. There are no significant intermolecular interactions, and acetonitrile solvent molecules simply occupy what would otherwise be voids in the structure.

## Experimental

All chemicals used were of analytical reagent grade and were used directly without further purification. A solution of $PPh_3$ (0.15 mg, 0.6 mmol) in acetonitrile (4 ml) was reacted with CuCl (0.03 mg, 0.3 mmol) in acetonitrile (5 ml). 1,2-Diaminopropane (0.02 mg, 0.3 mmol) in acetonitrile (3 ml) was added to the mixture, which was stirred for 1 h. Slow evaporation at room temperature of the solvent gave blue crystals.

## Refinement

The 1,2-diaminopropane ligand is twofold disordered, with refined occupancy factors of 0.599:0.401 (10); restraints were applied to the displacement parameters of this ligand. All H atoms were positioned geometrically, with N—H = 0.92 and C—H = 0.95–1.00 Å and $U_{iso}$(H) = 1.2$U_{eq}$(N,*C*) or 1.5$U_{eq}$(C) for methyl groups.

## Figures

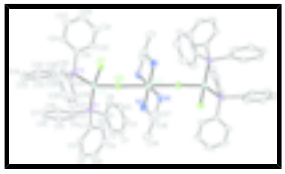


Fig. 1. The molecular structure with atom labels and 40% probability displacement ellipsoids. H atoms, solvent molecules, and the minor disorder components have been omitted. [Symmetry code for unlabelled atoms: $1-x$, $1-y$, $1-z$.]

## bis(1,2-diaminopropane-2κ$^2$*N*,*N*$^1$)di-μ-chlorido-1:2κ$^2$*Cl*,2:3κ$^2$*Cl*- dichlorido-1κ*Cl*,3κ*Cl*-tetrakis(triphenylphosphine)-1κ$^2$*P*,3κ$^2$*P*- tricopper(I,II,I) acetonitrile disolvate

*Crystal data*

| | |
|---|---|
| $[Cu_3Cl_4(C_3H_{10}N_2)_2(C_{18}H_{15}P_1)_4]\cdot 2C_2H_3N$ | $F_{000}$ = 1670 |
| $M_r$ = 1611.87 | $D_x$ = 1.353 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $a$ = 15.896 (3) Å | Cell parameters from 32758 reflections |
| $b$ = 9.4181 (15) Å | θ = 4.1–25.0º |
| $c$ = 26.533 (4) Å | μ = 1.06 mm$^{-1}$ |
| β = 94.957 (12)º | $T$ = 150 (2) K |
| $V$ = 3957.4 (11) Å$^3$ | Block, blue |
| $Z$ = 2 | 0.25 × 0.20 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD diffractometer | 6923 independent reflections |
| Radiation source: sealed tube | 5038 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.074 |
| $T$ = 150(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 4.1º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2007) | $h$ = −18→18 |
| $T_{min}$ = 0.780, $T_{max}$ = 0.820 | $k$ = −11→11 |
| 32758 measured reflections | $l$ = −31→31 |

*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 |
| $wR(F^2)$ = 0.158 | $w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 8.3144P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.03 | $(\Delta/\sigma)_{max} < 0.001$ |
| 6923 reflections | $\Delta\rho_{max}$ = 0.78 e Å$^{-3}$ |
| 496 parameters | $\Delta\rho_{min}$ = −0.81 e Å$^{-3}$ |
| 136 restraints | Extinction correction: SHELXTL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0032 (5) |

*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 | 0.28031 (3) | 0.32452 (6) | 0.389429 (19) | 0.02994 (19) | |
| Cl1 | 0.34277 (7) | 0.11509 (13) | 0.42371 (4) | 0.0381 (3) | |
| Cl2 | 0.39546 (7) | 0.49353 (13) | 0.40612 (5) | 0.0395 (3) | |
| P1 | 0.16988 (7) | 0.39615 (12) | 0.43263 (4) | 0.0267 (3) | |
| P2 | 0.26663 (7) | 0.29168 (13) | 0.30384 (4) | 0.0273 (3) | |
| C1 | 0.1891 (3) | 0.3852 (5) | 0.50241 (15) | 0.0291 (10) | |
| C2 | 0.1611 (3) | 0.4882 (5) | 0.53478 (17) | 0.0365 (11) | |
| H2 | 0.1327 | 0.5705 | 0.5213 | 0.044* | |
| C3 | 0.1750 (3) | 0.4699 (7) | 0.58722 (19) | 0.0505 (14) | |
| H3 | 0.1574 | 0.5410 | 0.6094 | 0.061* | |
| C4 | 0.2143 (3) | 0.3488 (7) | 0.60679 (18) | 0.0531 (15) | |
| H4 | 0.2225 | 0.3356 | 0.6424 | 0.064* | |
| C5 | 0.2418 (4) | 0.2472 (7) | 0.5747 (2) | 0.0585 (16) | |
| H5 | 0.2693 | 0.1645 | 0.5884 | 0.070* | |
| C6 | 0.2298 (3) | 0.2639 (6) | 0.52255 (17) | 0.0421 (12) | |
| H6 | 0.2491 | 0.1933 | 0.5007 | 0.050* | |
| C7 | 0.1373 (3) | 0.5817 (5) | 0.42317 (15) | 0.0308 (10) | |
| C8 | 0.2008 (3) | 0.6845 (5) | 0.42215 (18) | 0.0387 (12) | |
| H8 | 0.2583 | 0.6557 | 0.4240 | 0.046* | |
| C9 | 0.1808 (4) | 0.8288 (5) | 0.41839 (19) | 0.0436 (12) | |
| H9 | 0.2247 | 0.8974 | 0.4187 | 0.052* | |
| C10 | 0.0973 (3) | 0.8719 (5) | 0.41417 (17) | 0.0407 (12) | |
| H10 | 0.0839 | 0.9701 | 0.4116 | 0.049* | |
| C11 | 0.0332 (3) | 0.7719 (5) | 0.41377 (17) | 0.0394 (12) | |
| H11 | −0.0241 | 0.8015 | 0.4100 | 0.047* | |
| C12 | 0.0529 (3) | 0.6268 (5) | 0.41891 (16) | 0.0351 (11) | |
| H12 | 0.0088 | 0.5589 | 0.4195 | 0.042* | |
| C13 | 0.0702 (3) | 0.2987 (5) | 0.42097 (16) | 0.0285 (10) | |
| C14 | 0.0274 (3) | 0.2347 (5) | 0.45891 (17) | 0.0344 (11) | |
| H14 | 0.0496 | 0.2428 | 0.4932 | 0.041* | |
| C15 | −0.0471 (3) | 0.1590 (6) | 0.4472 (2) | 0.0447 (13) | |
| H15 | −0.0749 | 0.1154 | 0.4734 | 0.054* | |
| C16 | −0.0808 (3) | 0.1471 (6) | 0.3976 (2) | 0.0455 (13) | |

| | | | | | |
|---|---|---|---|---|---|
| H16 | −0.1314 | 0.0951 | 0.3898 | 0.055* | |
| C17 | −0.0399 (3) | 0.2120 (6) | 0.35907 (19) | 0.0439 (13) | |
| H17 | −0.0633 | 0.2059 | 0.3250 | 0.053* | |
| C18 | 0.0353 (3) | 0.2857 (5) | 0.37077 (17) | 0.0363 (11) | |
| H18 | 0.0633 | 0.3278 | 0.3443 | 0.044* | |
| C19 | 0.3537 (3) | 0.1937 (5) | 0.27892 (17) | 0.0332 (11) | |
| C20 | 0.4345 (3) | 0.2202 (6) | 0.3011 (2) | 0.0438 (12) | |
| H20 | 0.4421 | 0.2812 | 0.3297 | 0.053* | |
| C21 | 0.5043 (4) | 0.1580 (7) | 0.2818 (3) | 0.0645 (18) | |
| H21 | 0.5594 | 0.1769 | 0.2972 | 0.077* | |
| C22 | 0.4941 (4) | 0.0694 (7) | 0.2405 (3) | 0.0646 (18) | |
| H22 | 0.5422 | 0.0287 | 0.2272 | 0.078* | |
| C23 | 0.4144 (4) | 0.0390 (6) | 0.2182 (2) | 0.0527 (15) | |
| H23 | 0.4074 | −0.0221 | 0.1897 | 0.063* | |
| C24 | 0.3441 (3) | 0.0994 (5) | 0.23824 (17) | 0.0407 (12) | |
| H24 | 0.2890 | 0.0759 | 0.2239 | 0.049* | |
| C25 | 0.2624 (3) | 0.4519 (5) | 0.26432 (17) | 0.0317 (10) | |
| C26 | 0.2333 (3) | 0.5768 (6) | 0.2848 (2) | 0.0460 (13) | |
| H26 | 0.2168 | 0.5776 | 0.3184 | 0.055* | |
| C27 | 0.2282 (4) | 0.7010 (6) | 0.2559 (3) | 0.0637 (17) | |
| H27 | 0.2093 | 0.7864 | 0.2703 | 0.076* | |
| C28 | 0.2503 (4) | 0.7013 (6) | 0.2066 (2) | 0.0577 (16) | |
| H28 | 0.2451 | 0.7855 | 0.1869 | 0.069* | |
| C29 | 0.2798 (3) | 0.5784 (6) | 0.1865 (2) | 0.0467 (13) | |
| H29 | 0.2954 | 0.5781 | 0.1528 | 0.056* | |
| C30 | 0.2870 (3) | 0.4546 (6) | 0.21499 (17) | 0.0399 (12) | |
| H30 | 0.3089 | 0.3711 | 0.2008 | 0.048* | |
| C31 | 0.1742 (3) | 0.1909 (5) | 0.27813 (15) | 0.0278 (10) | |
| C32 | 0.1217 (3) | 0.2291 (5) | 0.23523 (16) | 0.0349 (11) | |
| H32 | 0.1331 | 0.3129 | 0.2171 | 0.042* | |
| C33 | 0.0521 (3) | 0.1441 (6) | 0.21885 (19) | 0.0479 (14) | |
| H33 | 0.0172 | 0.1700 | 0.1894 | 0.057* | |
| C34 | 0.0340 (3) | 0.0232 (6) | 0.24513 (19) | 0.0453 (13) | |
| H34 | −0.0135 | −0.0334 | 0.2340 | 0.054* | |
| C35 | 0.0852 (3) | −0.0154 (6) | 0.28761 (19) | 0.0445 (13) | |
| H35 | 0.0730 | −0.0991 | 0.3056 | 0.053* | |
| C36 | 0.1539 (3) | 0.0669 (5) | 0.30402 (18) | 0.0384 (11) | |
| H36 | 0.1883 | 0.0393 | 0.3334 | 0.046* | |
| Cu2 | 0.5000 | 0.5000 | 0.5000 | 0.0436 (3) | |
| N1 | 0.5266 (6) | 0.7108 (10) | 0.4930 (4) | 0.044 (2) | 0.599 (10) |
| H1A | 0.5707 | 0.7364 | 0.5160 | 0.053* | 0.599 (10) |
| H1B | 0.5416 | 0.7300 | 0.4610 | 0.053* | 0.599 (10) |
| N2 | 0.3990 (6) | 0.5691 (12) | 0.5324 (4) | 0.051 (2) | 0.599 (10) |
| H2A | 0.3511 | 0.5558 | 0.5109 | 0.061* | 0.599 (10) |
| H2B | 0.3931 | 0.5189 | 0.5616 | 0.061* | 0.599 (10) |
| C37 | 0.4493 (8) | 0.7906 (14) | 0.5028 (5) | 0.063 (3) | 0.599 (10) |
| H37A | 0.4639 | 0.8903 | 0.5115 | 0.076* | 0.599 (10) |
| H37B | 0.4093 | 0.7906 | 0.4721 | 0.076* | 0.599 (10) |
| C38 | 0.4101 (14) | 0.724 (2) | 0.5445 (6) | 0.061 (4) | 0.599 (10) |

| | | | | | |
|---|---|---|---|---|---|
| H38 | 0.4493 | 0.7336 | 0.5758 | 0.073* | 0.599 (10) |
| C39 | 0.3253 (7) | 0.7951 (13) | 0.5539 (5) | 0.081 (4) | 0.599 (10) |
| H39A | 0.3009 | 0.7473 | 0.5820 | 0.121* | 0.599 (10) |
| H39B | 0.2863 | 0.7876 | 0.5233 | 0.121* | 0.599 (10) |
| H39C | 0.3349 | 0.8954 | 0.5623 | 0.121* | 0.599 (10) |
| N1X | 0.3985 (9) | 0.4925 (18) | 0.5435 (6) | 0.053 (4) | 0.401 (10) |
| H1X1 | 0.3505 | 0.4650 | 0.5241 | 0.064* | 0.401 (10) |
| H1X2 | 0.4086 | 0.4281 | 0.5694 | 0.064* | 0.401 (10) |
| N2X | 0.4906 (10) | 0.7100 (19) | 0.5076 (6) | 0.049 (3) | 0.401 (10) |
| H2X1 | 0.5319 | 0.7425 | 0.5312 | 0.059* | 0.401 (10) |
| H2X2 | 0.4973 | 0.7540 | 0.4773 | 0.059* | 0.401 (10) |
| C37X | 0.3874 (12) | 0.634 (2) | 0.5640 (9) | 0.078 (5) | 0.401 (10) |
| H37C | 0.4273 | 0.6486 | 0.5943 | 0.094* | 0.401 (10) |
| H37D | 0.3292 | 0.6444 | 0.5742 | 0.094* | 0.401 (10) |
| C38X | 0.403 (2) | 0.743 (3) | 0.5247 (10) | 0.064 (5) | 0.401 (10) |
| H38X | 0.3595 | 0.7334 | 0.4953 | 0.077* | 0.401 (10) |
| C39X | 0.3998 (12) | 0.8929 (17) | 0.5458 (6) | 0.072 (5) | 0.401 (10) |
| H39D | 0.4107 | 0.9613 | 0.5193 | 0.108* | 0.401 (10) |
| H39E | 0.4428 | 0.9031 | 0.5743 | 0.108* | 0.401 (10) |
| H39F | 0.3438 | 0.9106 | 0.5573 | 0.108* | 0.401 (10) |
| N3 | 0.4423 (5) | 0.3375 (13) | 0.1140 (3) | 0.156 (4) | |
| C40 | 0.5077 (5) | 0.3358 (9) | 0.1341 (3) | 0.078 (2) | |
| C41 | 0.5903 (4) | 0.3360 (6) | 0.1589 (2) | 0.0524 (14) | |
| H41A | 0.6241 | 0.4097 | 0.1442 | 0.079* | |
| H41B | 0.6166 | 0.2431 | 0.1547 | 0.079* | |
| H41C | 0.5873 | 0.3552 | 0.1950 | 0.079* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0258 (3) | 0.0369 (4) | 0.0267 (3) | 0.0007 (2) | −0.0002 (2) | −0.0018 (2) |
| Cl1 | 0.0391 (6) | 0.0331 (7) | 0.0417 (6) | 0.0027 (5) | 0.0009 (5) | 0.0013 (5) |
| Cl2 | 0.0340 (6) | 0.0369 (7) | 0.0455 (7) | −0.0061 (5) | −0.0079 (5) | 0.0000 (5) |
| P1 | 0.0257 (6) | 0.0294 (7) | 0.0248 (6) | 0.0016 (5) | 0.0008 (4) | −0.0004 (5) |
| P2 | 0.0255 (6) | 0.0317 (7) | 0.0244 (6) | 0.0028 (5) | 0.0000 (4) | −0.0001 (5) |
| C1 | 0.025 (2) | 0.039 (3) | 0.023 (2) | −0.001 (2) | 0.0002 (17) | 0.0017 (19) |
| C2 | 0.031 (2) | 0.043 (3) | 0.035 (3) | 0.005 (2) | 0.000 (2) | −0.006 (2) |
| C3 | 0.046 (3) | 0.071 (4) | 0.035 (3) | 0.002 (3) | 0.003 (2) | −0.017 (3) |
| C4 | 0.048 (3) | 0.086 (5) | 0.024 (2) | 0.007 (3) | −0.006 (2) | −0.001 (3) |
| C5 | 0.062 (4) | 0.073 (4) | 0.039 (3) | 0.026 (3) | 0.002 (3) | 0.014 (3) |
| C6 | 0.046 (3) | 0.051 (3) | 0.029 (2) | 0.014 (3) | −0.001 (2) | −0.002 (2) |
| C7 | 0.031 (2) | 0.037 (3) | 0.025 (2) | 0.001 (2) | 0.0013 (18) | −0.0037 (19) |
| C8 | 0.036 (3) | 0.037 (3) | 0.043 (3) | −0.003 (2) | −0.001 (2) | 0.000 (2) |
| C9 | 0.056 (3) | 0.028 (3) | 0.048 (3) | −0.003 (2) | 0.009 (2) | 0.003 (2) |
| C10 | 0.059 (3) | 0.028 (3) | 0.035 (3) | 0.009 (2) | 0.008 (2) | 0.001 (2) |
| C11 | 0.044 (3) | 0.040 (3) | 0.035 (3) | 0.013 (2) | 0.006 (2) | 0.002 (2) |
| C12 | 0.035 (3) | 0.037 (3) | 0.034 (2) | 0.002 (2) | 0.0015 (19) | −0.001 (2) |
| C13 | 0.026 (2) | 0.025 (3) | 0.035 (2) | 0.0035 (18) | 0.0023 (18) | −0.0012 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.036 (3) | 0.038 (3) | 0.029 (2) | 0.000 (2) | −0.0010 (19) | −0.002 (2) |
| C15 | 0.034 (3) | 0.048 (3) | 0.053 (3) | −0.005 (2) | 0.009 (2) | 0.002 (2) |
| C16 | 0.027 (2) | 0.052 (3) | 0.057 (3) | −0.004 (2) | 0.002 (2) | −0.011 (3) |
| C17 | 0.036 (3) | 0.056 (3) | 0.038 (3) | 0.007 (2) | −0.005 (2) | −0.010 (2) |
| C18 | 0.029 (2) | 0.048 (3) | 0.032 (2) | 0.005 (2) | −0.0004 (19) | −0.002 (2) |
| C19 | 0.035 (3) | 0.034 (3) | 0.032 (2) | 0.008 (2) | 0.0057 (19) | 0.009 (2) |
| C20 | 0.030 (3) | 0.041 (3) | 0.061 (3) | 0.001 (2) | 0.005 (2) | −0.001 (3) |
| C21 | 0.029 (3) | 0.050 (4) | 0.116 (6) | 0.004 (3) | 0.017 (3) | −0.002 (4) |
| C22 | 0.045 (4) | 0.055 (4) | 0.099 (5) | 0.017 (3) | 0.038 (3) | 0.007 (4) |
| C23 | 0.060 (4) | 0.048 (4) | 0.052 (3) | 0.021 (3) | 0.016 (3) | −0.001 (3) |
| C24 | 0.042 (3) | 0.047 (3) | 0.032 (2) | 0.016 (2) | 0.000 (2) | 0.001 (2) |
| C25 | 0.030 (2) | 0.028 (3) | 0.036 (2) | 0.002 (2) | −0.0036 (19) | 0.001 (2) |
| C26 | 0.045 (3) | 0.044 (3) | 0.048 (3) | 0.006 (2) | −0.001 (2) | −0.003 (2) |
| C27 | 0.064 (4) | 0.035 (4) | 0.089 (5) | 0.010 (3) | −0.007 (3) | −0.001 (3) |
| C28 | 0.051 (3) | 0.046 (4) | 0.071 (4) | −0.007 (3) | −0.021 (3) | 0.023 (3) |
| C29 | 0.046 (3) | 0.048 (4) | 0.045 (3) | −0.010 (3) | −0.006 (2) | 0.011 (3) |
| C30 | 0.040 (3) | 0.044 (3) | 0.034 (3) | −0.003 (2) | −0.003 (2) | 0.004 (2) |
| C31 | 0.026 (2) | 0.032 (3) | 0.026 (2) | 0.0050 (19) | 0.0030 (17) | −0.0022 (18) |
| C32 | 0.033 (3) | 0.040 (3) | 0.030 (2) | 0.002 (2) | −0.0031 (19) | −0.002 (2) |
| C33 | 0.044 (3) | 0.066 (4) | 0.033 (3) | −0.002 (3) | −0.007 (2) | −0.010 (3) |
| C34 | 0.041 (3) | 0.050 (3) | 0.045 (3) | −0.013 (2) | 0.002 (2) | −0.013 (3) |
| C35 | 0.050 (3) | 0.039 (3) | 0.044 (3) | −0.009 (2) | 0.004 (2) | −0.006 (2) |
| C36 | 0.041 (3) | 0.037 (3) | 0.037 (3) | 0.001 (2) | 0.002 (2) | 0.000 (2) |
| Cu2 | 0.0374 (5) | 0.0428 (6) | 0.0508 (5) | −0.0041 (4) | 0.0044 (4) | −0.0060 (4) |
| N1 | 0.033 (5) | 0.055 (5) | 0.042 (5) | −0.003 (4) | −0.003 (4) | 0.005 (4) |
| N2 | 0.050 (5) | 0.049 (6) | 0.055 (6) | −0.020 (5) | 0.016 (4) | −0.011 (5) |
| C37 | 0.054 (7) | 0.053 (7) | 0.084 (8) | 0.002 (5) | 0.012 (5) | 0.005 (6) |
| C38 | 0.069 (7) | 0.056 (8) | 0.060 (9) | 0.006 (6) | 0.019 (7) | −0.010 (7) |
| C39 | 0.071 (7) | 0.080 (8) | 0.095 (9) | −0.001 (6) | 0.026 (6) | −0.036 (7) |
| N1X | 0.042 (7) | 0.061 (8) | 0.057 (8) | −0.023 (8) | 0.008 (6) | 0.008 (7) |
| N2X | 0.035 (8) | 0.061 (9) | 0.051 (8) | −0.009 (7) | 0.004 (6) | −0.003 (6) |
| C37X | 0.070 (10) | 0.065 (8) | 0.106 (13) | −0.001 (9) | 0.040 (9) | 0.006 (9) |
| C38X | 0.067 (10) | 0.054 (8) | 0.076 (14) | 0.007 (9) | 0.030 (12) | −0.005 (9) |
| C39X | 0.098 (14) | 0.059 (8) | 0.057 (9) | 0.018 (9) | −0.001 (8) | 0.001 (7) |
| N3 | 0.065 (5) | 0.265 (13) | 0.133 (7) | −0.008 (6) | −0.014 (5) | −0.021 (7) |
| C40 | 0.057 (4) | 0.117 (6) | 0.059 (4) | −0.009 (4) | 0.001 (3) | −0.007 (4) |
| C41 | 0.056 (3) | 0.048 (4) | 0.053 (3) | −0.006 (3) | 0.001 (3) | −0.005 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—Cl1 | 2.3553 (13) | C28—H28 | 0.950 |
| Cu1—Cl2 | 2.4372 (13) | C28—C29 | 1.374 (8) |
| Cu1—P1 | 2.2800 (13) | C29—H29 | 0.950 |
| Cu1—P2 | 2.2835 (12) | C29—C30 | 1.388 (7) |
| P1—C1 | 1.853 (4) | C30—H30 | 0.950 |
| P1—C7 | 1.834 (5) | C31—C32 | 1.400 (6) |
| P1—C13 | 1.834 (4) | C31—C36 | 1.406 (7) |
| P2—C19 | 1.834 (5) | C32—H32 | 0.950 |
| P2—C25 | 1.836 (5) | C32—C33 | 1.403 (7) |

| | | | |
|---|---|---|---|
| P2—C31 | 1.830 (4) | C33—H33 | 0.950 |
| C1—C2 | 1.394 (6) | C33—C34 | 1.378 (8) |
| C1—C6 | 1.396 (7) | C34—H34 | 0.950 |
| C2—H2 | 0.950 | C34—C35 | 1.381 (7) |
| C2—C3 | 1.401 (7) | C35—H35 | 0.950 |
| C3—H3 | 0.950 | C35—C36 | 1.379 (7) |
| C3—C4 | 1.380 (8) | C36—H36 | 0.950 |
| C4—H4 | 0.950 | Cu2—Cl2 | 2.8731 (12) |
| C4—C5 | 1.377 (8) | Cu2—Cl2$^{i}$ | 2.8731 (12) |
| C5—H5 | 0.950 | Cu2—N1 | 2.042 (10) |
| C5—C6 | 1.388 (7) | Cu2—N1$^{i}$ | 2.042 (10) |
| C6—H6 | 0.950 | Cu2—N2 | 1.995 (10) |
| C7—C8 | 1.400 (7) | Cu2—N2$^{i}$ | 1.995 (10) |
| C7—C12 | 1.402 (6) | Cu2—N1X | 2.065 (14) |
| C8—H8 | 0.950 | Cu2—N1X$^{i}$ | 2.065 (14) |
| C8—C9 | 1.397 (7) | Cu2—N2X | 1.995 (18) |
| C9—H9 | 0.950 | Cu2—N2X$^{i}$ | 1.995 (18) |
| C9—C10 | 1.383 (7) | N1—H1A | 0.920 |
| C10—H10 | 0.950 | N1—H1B | 0.920 |
| C10—C11 | 1.388 (7) | N1—C37 | 1.482 (15) |
| C11—H11 | 0.950 | N2—H2A | 0.920 |
| C11—C12 | 1.406 (7) | N2—H2B | 0.920 |
| C12—H12 | 0.950 | N2—C38 | 1.50 (2) |
| C13—C14 | 1.399 (6) | C37—H37A | 0.990 |
| C13—C18 | 1.404 (6) | C37—H37B | 0.990 |
| C14—H14 | 0.950 | C37—C38 | 1.46 (2) |
| C14—C15 | 1.395 (7) | C38—H38 | 1.000 |
| C15—H15 | 0.950 | C38—C39 | 1.54 (2) |
| C15—C16 | 1.380 (7) | C39—H39A | 0.980 |
| C16—H16 | 0.950 | C39—H39B | 0.980 |
| C16—C17 | 1.400 (7) | C39—H39C | 0.980 |
| C17—H17 | 0.950 | N1X—H1X1 | 0.920 |
| C17—C18 | 1.393 (7) | N1X—H1X2 | 0.920 |
| C18—H18 | 0.950 | N1X—C37X | 1.46 (2) |
| C19—C20 | 1.388 (7) | N2X—H2X1 | 0.920 |
| C19—C24 | 1.396 (7) | N2X—H2X2 | 0.920 |
| C20—H20 | 0.950 | N2X—C38X | 1.54 (3) |
| C20—C21 | 1.392 (7) | C37X—H37C | 0.990 |
| C21—H21 | 0.950 | C37X—H37D | 0.990 |
| C21—C22 | 1.376 (9) | C37X—C38X | 1.50 (3) |
| C22—H22 | 0.950 | C38X—H38X | 1.000 |
| C22—C23 | 1.381 (9) | C38X—C39X | 1.52 (3) |
| C23—H23 | 0.950 | C39X—H39D | 0.980 |
| C23—C24 | 1.399 (7) | C39X—H39E | 0.980 |
| C24—H24 | 0.950 | C39X—H39F | 0.980 |
| C25—C26 | 1.392 (7) | N3—C40 | 1.127 (9) |
| C25—C30 | 1.398 (7) | C40—C41 | 1.417 (9) |
| C26—H26 | 0.950 | C41—H41A | 0.980 |

| | | | |
|---|---|---|---|
| C26—C27 | 1.397 (8) | C41—H41B | 0.980 |
| C27—H27 | 0.950 | C41—H41C | 0.980 |
| C27—C28 | 1.382 (9) | | |
| Cl1—Cu1—Cl2 | 101.06 (5) | C31—C32—H32 | 119.9 |
| Cl1—Cu1—P1 | 111.76 (5) | C31—C32—C33 | 120.3 (5) |
| Cl1—Cu1—P2 | 105.75 (5) | H32—C32—C33 | 119.9 |
| Cl2—Cu1—P1 | 108.31 (5) | C32—C33—H33 | 119.7 |
| Cl2—Cu1—P2 | 105.94 (5) | C32—C33—C34 | 120.5 (5) |
| P1—Cu1—P2 | 121.92 (4) | H33—C33—C34 | 119.7 |
| Cu1—Cl2—Cu2 | 122.71 (5) | C33—C34—H34 | 120.1 |
| Cu1—P1—C1 | 114.74 (14) | C33—C34—C35 | 119.8 (5) |
| Cu1—P1—C7 | 115.70 (15) | H34—C34—C35 | 120.1 |
| Cu1—P1—C13 | 117.30 (14) | C34—C35—H35 | 119.9 |
| C1—P1—C7 | 102.1 (2) | C34—C35—C36 | 120.3 (5) |
| C1—P1—C13 | 101.9 (2) | H35—C35—C36 | 119.9 |
| C7—P1—C13 | 102.9 (2) | C31—C36—C35 | 121.4 (4) |
| Cu1—P2—C19 | 114.63 (15) | C31—C36—H36 | 119.3 |
| Cu1—P2—C25 | 116.89 (15) | C35—C36—H36 | 119.3 |
| Cu1—P2—C31 | 116.44 (14) | Cl2—Cu2—Cl2$^{i}$ | 180.0 |
| C19—P2—C25 | 101.5 (2) | Cl2—Cu2—N1 | 92.9 (3) |
| C19—P2—C31 | 102.2 (2) | Cl2$^{i}$—Cu2—N1$^{i}$ | 92.9 (3) |
| C25—P2—C31 | 103.0 (2) | Cl2$^{i}$—Cu2—N1 | 87.1 (3) |
| P1—C1—C2 | 122.9 (3) | Cl2—Cu2—N1$^{i}$ | 87.1 (3) |
| P1—C1—C6 | 117.3 (3) | Cl2—Cu2—N2 | 87.4 (3) |
| C2—C1—C6 | 119.7 (4) | Cl2$^{i}$—Cu2—N2$^{i}$ | 87.4 (3) |
| C1—C2—H2 | 120.2 | Cl2$^{i}$—Cu2—N2 | 92.6 (3) |
| C1—C2—C3 | 119.6 (5) | Cl2—Cu2—N2$^{i}$ | 92.6 (3) |
| H2—C2—C3 | 120.2 | Cl2—Cu2—N1X | 93.6 (4) |
| C2—C3—H3 | 119.9 | Cl2$^{i}$—Cu2—N1X$^{i}$ | 93.6 (4) |
| C2—C3—C4 | 120.2 (5) | Cl2$^{i}$—Cu2—N1X | 86.4 (4) |
| H3—C3—C4 | 119.9 | Cl2—Cu2—N1X$^{i}$ | 86.4 (4) |
| C3—C4—H4 | 120.0 | Cl2—Cu2—N2X | 93.8 (5) |
| C3—C4—C5 | 119.9 (5) | Cl2$^{i}$—Cu2—N2X$^{i}$ | 93.8 (5) |
| H4—C4—C5 | 120.0 | Cl2$^{i}$—Cu2—N2X | 86.2 (5) |
| C4—C5—H5 | 119.5 | Cl2—Cu2—N2X$^{i}$ | 86.2 (5) |
| C4—C5—C6 | 121.0 (5) | N1—Cu2—N1$^{i}$ | 180.0 |
| H5—C5—C6 | 119.5 | N1—Cu2—N2 | 84.4 (4) |
| C1—C6—C5 | 119.5 (5) | N1$^{i}$—Cu2—N2$^{i}$ | 84.4 (4) |
| C1—C6—H6 | 120.2 | N1$^{i}$—Cu2—N2 | 95.6 (4) |
| C5—C6—H6 | 120.2 | N1—Cu2—N2$^{i}$ | 95.6 (4) |
| P1—C7—C8 | 117.8 (3) | N2—Cu2—N2$^{i}$ | 180.0 |
| P1—C7—C12 | 123.8 (4) | N1X—Cu2—N1X$^{i}$ | 180.0 |
| C8—C7—C12 | 118.4 (4) | N1X—Cu2—N2X | 84.7 (6) |
| C7—C8—H8 | 119.5 | N1X$^{i}$—Cu2—N2X$^{i}$ | 84.7 (6) |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 120.9 (5) | N1X$^{i}$—Cu2—N2X | 95.3 (6) |
| H8—C8—C9 | 119.5 | N1X—Cu2—N2X$^{i}$ | 95.3 (6) |
| C8—C9—H9 | 120.0 | N2X—Cu2—N2X$^{i}$ | 180.0 |
| C8—C9—C10 | 120.1 (5) | Cu2—N1—H1A | 110.3 |
| H9—C9—C10 | 120.0 | Cu2—N1—H1B | 110.3 |
| C9—C10—H10 | 120.0 | Cu2—N1—C37 | 107.2 (7) |
| C9—C10—C11 | 120.0 (5) | H1A—N1—H1B | 108.5 |
| H10—C10—C11 | 120.0 | H1A—N1—C37 | 110.3 |
| C10—C11—H11 | 119.9 | H1B—N1—C37 | 110.3 |
| C10—C11—C12 | 120.1 (5) | Cu2—N2—H2A | 109.9 |
| H11—C11—C12 | 119.9 | Cu2—N2—H2B | 109.9 |
| C7—C12—C11 | 120.4 (5) | Cu2—N2—C38 | 108.9 (10) |
| C7—C12—H12 | 119.8 | H2A—N2—H2B | 108.3 |
| C11—C12—H12 | 119.8 | H2A—N2—C38 | 109.9 |
| P1—C13—C14 | 124.1 (3) | H2B—N2—C38 | 109.9 |
| P1—C13—C18 | 118.0 (3) | N1—C37—H37A | 109.8 |
| C14—C13—C18 | 117.9 (4) | N1—C37—H37B | 109.8 |
| C13—C14—H14 | 119.5 | N1—C37—C38 | 109.3 (12) |
| C13—C14—C15 | 121.1 (4) | H37A—C37—H37B | 108.3 |
| H14—C14—C15 | 119.5 | H37A—C37—C38 | 109.8 |
| C14—C15—H15 | 119.8 | H37B—C37—C38 | 109.8 |
| C14—C15—C16 | 120.4 (5) | N2—C38—C37 | 107.9 (13) |
| H15—C15—C16 | 119.8 | N2—C38—H38 | 108.5 |
| C15—C16—H16 | 120.2 | N2—C38—C39 | 111.5 (15) |
| C15—C16—C17 | 119.6 (5) | C37—C38—H38 | 108.5 |
| H16—C16—C17 | 120.2 | C37—C38—C39 | 111.9 (14) |
| C16—C17—H17 | 120.1 | H38—C38—C39 | 108.5 |
| C16—C17—C18 | 119.9 (4) | C38—C39—H39A | 109.5 |
| H17—C17—C18 | 120.1 | C38—C39—H39B | 109.5 |
| C13—C18—C17 | 121.1 (4) | C38—C39—H39C | 109.5 |
| C13—C18—H18 | 119.4 | H39A—C39—H39B | 109.5 |
| C17—C18—H18 | 119.4 | H39A—C39—H39C | 109.5 |
| P2—C19—C20 | 117.1 (4) | H39B—C39—H39C | 109.5 |
| P2—C19—C24 | 124.3 (4) | Cu2—N1X—H1X1 | 110.2 |
| C20—C19—C24 | 118.6 (4) | Cu2—N1X—H1X2 | 110.2 |
| C19—C20—H20 | 119.8 | Cu2—N1X—C37X | 107.6 (11) |
| C19—C20—C21 | 120.4 (5) | H1X1—N1X—H1X2 | 108.5 |
| H20—C20—C21 | 119.8 | H1X1—N1X—C37X | 110.2 |
| C20—C21—H21 | 119.8 | H1X2—N1X—C37X | 110.2 |
| C20—C21—C22 | 120.3 (6) | Cu2—N2X—H2X1 | 110.1 |
| H21—C21—C22 | 119.8 | Cu2—N2X—H2X2 | 110.1 |
| C21—C22—H22 | 119.7 | Cu2—N2X—C38X | 108.1 (14) |
| C21—C22—C23 | 120.5 (5) | H2X1—N2X—H2X2 | 108.4 |
| H22—C22—C23 | 119.7 | H2X1—N2X—C38X | 110.1 |
| C22—C23—H23 | 120.4 | H2X2—N2X—C38X | 110.1 |
| C22—C23—C24 | 119.2 (5) | N1X—C37X—H37C | 109.7 |
| H23—C23—C24 | 120.4 | N1X—C37X—H37D | 109.7 |
| C19—C24—C23 | 120.9 (5) | N1X—C37X—C38X | 110 (2) |

| | | | |
|---|---|---|---|
| C19—C24—H24 | 119.5 | H37C—C37X—H37D | 108.2 |
| C23—C24—H24 | 119.5 | H37C—C37X—C38X | 109.7 |
| P2—C25—C26 | 117.9 (4) | H37D—C37X—C38X | 109.7 |
| P2—C25—C30 | 123.4 (4) | N2X—C38X—C37X | 106 (2) |
| C26—C25—C30 | 118.7 (5) | N2X—C38X—H38X | 109.4 |
| C25—C26—H26 | 120.1 | N2X—C38X—C39X | 111 (2) |
| C25—C26—C27 | 119.9 (5) | C37X—C38X—H38X | 109.4 |
| H26—C26—C27 | 120.1 | C37X—C38X—C39X | 112 (2) |
| C26—C27—H27 | 119.6 | H38X—C38X—C39X | 109.4 |
| C26—C27—C28 | 120.9 (6) | C38X—C39X—H39D | 109.5 |
| H27—C27—C28 | 119.6 | C38X—C39X—H39E | 109.5 |
| C27—C28—H28 | 120.4 | C38X—C39X—H39F | 109.5 |
| C27—C28—C29 | 119.2 (5) | H39D—C39X—H39E | 109.5 |
| H28—C28—C29 | 120.4 | H39D—C39X—H39F | 109.5 |
| C28—C29—H29 | 119.6 | H39E—C39X—H39F | 109.5 |
| C28—C29—C30 | 120.7 (5) | N3—C40—C41 | 179.0 (11) |
| H29—C29—C30 | 119.6 | C40—C41—H41A | 109.5 |
| C25—C30—C29 | 120.5 (5) | C40—C41—H41B | 109.5 |
| C25—C30—H30 | 119.7 | C40—C41—H41C | 109.5 |
| C29—C30—H30 | 119.7 | H41A—C41—H41B | 109.5 |
| P2—C31—C32 | 125.0 (4) | H41A—C41—H41C | 109.5 |
| P2—C31—C36 | 117.3 (3) | H41B—C41—H41C | 109.5 |
| C32—C31—C36 | 117.7 (4) | | |
| Cl1—Cu1—Cl2—Cu2 | −42.00 (6) | C24—C19—C20—C21 | 2.4 (8) |
| P1—Cu1—Cl2—Cu2 | 75.56 (6) | C19—C20—C21—C22 | −0.1 (9) |
| P2—Cu1—Cl2—Cu2 | −152.08 (5) | C20—C21—C22—C23 | −1.1 (10) |
| Cl1—Cu1—P1—C1 | 43.17 (17) | C21—C22—C23—C24 | −0.1 (9) |
| Cl1—Cu1—P1—C7 | 161.75 (15) | P2—C19—C24—C23 | 173.8 (4) |
| Cl1—Cu1—P1—C13 | −76.36 (16) | C20—C19—C24—C23 | −3.7 (7) |
| Cl2—Cu1—P1—C1 | −67.31 (17) | C22—C23—C24—C19 | 2.5 (8) |
| Cl2—Cu1—P1—C7 | 51.28 (16) | Cu1—P2—C25—C26 | −26.0 (4) |
| Cl2—Cu1—P1—C13 | 173.17 (16) | Cu1—P2—C25—C30 | 154.0 (3) |
| P2—Cu1—P1—C1 | 169.53 (17) | C19—P2—C25—C26 | −151.4 (4) |
| P2—Cu1—P1—C7 | −71.88 (16) | C19—P2—C25—C30 | 28.6 (4) |
| P2—Cu1—P1—C13 | 50.00 (17) | C31—P2—C25—C26 | 103.1 (4) |
| Cl1—Cu1—P2—C19 | −36.71 (18) | C31—P2—C25—C30 | −77.0 (4) |
| Cl1—Cu1—P2—C25 | −155.27 (17) | P2—C25—C26—C27 | −179.3 (4) |
| Cl1—Cu1—P2—C31 | 82.45 (16) | C30—C25—C26—C27 | 0.7 (7) |
| Cl2—Cu1—P2—C19 | 70.02 (18) | C25—C26—C27—C28 | 1.2 (9) |
| Cl2—Cu1—P2—C25 | −48.54 (17) | C26—C27—C28—C29 | −1.8 (9) |
| Cl2—Cu1—P2—C31 | −170.83 (16) | C27—C28—C29—C30 | 0.4 (8) |
| P1—Cu1—P2—C19 | −165.73 (17) | C28—C29—C30—C25 | 1.6 (8) |
| P1—Cu1—P2—C25 | 75.71 (17) | P2—C25—C30—C29 | 178.0 (4) |
| P1—Cu1—P2—C31 | −46.57 (17) | C26—C25—C30—C29 | −2.1 (7) |
| Cu1—P1—C1—C2 | 140.6 (3) | Cu1—P2—C31—C32 | 134.9 (3) |
| Cu1—P1—C1—C6 | −42.7 (4) | Cu1—P2—C31—C36 | −44.1 (4) |
| C7—P1—C1—C2 | 14.6 (4) | C19—P2—C31—C32 | −99.4 (4) |
| C7—P1—C1—C6 | −168.7 (4) | C19—P2—C31—C36 | 81.6 (4) |
| C13—P1—C1—C2 | −91.6 (4) | C25—P2—C31—C32 | 5.6 (4) |

| | | | |
|---|---|---|---|
| C13—P1—C1—C6 | 85.1 (4) | C25—P2—C31—C36 | −173.4 (3) |
| P1—C1—C2—C3 | 177.5 (4) | P2—C31—C32—C33 | −179.8 (4) |
| C6—C1—C2—C3 | 0.8 (7) | C36—C31—C32—C33 | −0.9 (7) |
| C1—C2—C3—C4 | −1.6 (8) | C31—C32—C33—C34 | 0.9 (8) |
| C2—C3—C4—C5 | 1.5 (9) | C32—C33—C34—C35 | −0.7 (8) |
| C3—C4—C5—C6 | −0.6 (9) | C33—C34—C35—C36 | 0.4 (8) |
| C4—C5—C6—C1 | −0.2 (9) | C34—C35—C36—C31 | −0.4 (8) |
| P1—C1—C6—C5 | −176.7 (4) | P2—C31—C36—C35 | 179.7 (4) |
| C2—C1—C6—C5 | 0.1 (7) | C32—C31—C36—C35 | 0.6 (7) |
| Cu1—P1—C7—C8 | −41.7 (4) | Cu1—Cl2—Cu2—N1 | −153.1 (3) |
| Cu1—P1—C7—C12 | 140.8 (3) | Cu1—Cl2—Cu2—N1$^{i}$ | 26.9 (3) |
| C1—P1—C7—C8 | 83.6 (4) | Cu1—Cl2—Cu2—N2 | −68.8 (3) |
| C1—P1—C7—C12 | −93.8 (4) | Cu1—Cl2—Cu2—N2$^{i}$ | 111.2 (3) |
| C13—P1—C7—C8 | −171.0 (3) | Cu1—Cl2—Cu2—N1X | −47.7 (5) |
| C13—P1—C7—C12 | 11.6 (4) | Cu1—Cl2—Cu2—N1X$^{i}$ | 132.3 (5) |
| P1—C7—C8—C9 | −175.8 (4) | Cu1—Cl2—Cu2—N2X | −132.6 (5) |
| C12—C7—C8—C9 | 1.8 (7) | Cu1—Cl2—Cu2—N2X$^{i}$ | 47.4 (5) |
| C7—C8—C9—C10 | −1.8 (7) | Cl2—Cu2—N1—C37 | 73.0 (7) |
| C8—C9—C10—C11 | 0.1 (7) | Cl2$^{i}$—Cu2—N1—C37 | −107.0 (7) |
| C9—C10—C11—C12 | 1.6 (7) | N2—Cu2—N1—C37 | −14.1 (7) |
| P1—C7—C12—C11 | 177.4 (3) | N2$^{i}$—Cu2—N1—C37 | 165.9 (7) |
| C8—C7—C12—C11 | 0.0 (6) | Cl2—Cu2—N2—C38 | −106.5 (9) |
| C10—C11—C12—C7 | −1.6 (7) | Cl2$^{i}$—Cu2—N2—C38 | 73.5 (9) |
| Cu1—P1—C13—C14 | 124.8 (4) | N1—Cu2—N2—C38 | −13.3 (9) |
| Cu1—P1—C13—C18 | −54.2 (4) | N1$^{i}$—Cu2—N2—C38 | 166.7 (9) |
| C1—P1—C13—C14 | −1.3 (4) | Cu2—N1—C37—C38 | 40.1 (12) |
| C1—P1—C13—C18 | 179.7 (4) | N1—C37—C38—N2 | −52.5 (16) |
| C7—P1—C13—C14 | −106.9 (4) | N1—C37—C38—C39 | −175.5 (11) |
| C7—P1—C13—C18 | 74.1 (4) | Cu2—N2—C38—C37 | 39.0 (15) |
| P1—C13—C14—C15 | −178.3 (4) | Cu2—N2—C38—C39 | 162.3 (9) |
| C18—C13—C14—C15 | 0.6 (7) | Cl2—Cu2—N1X—C37X | −104.8 (12) |
| C13—C14—C15—C16 | −0.7 (8) | Cl2$^{i}$—Cu2—N1X—C37X | 75.2 (12) |
| C14—C15—C16—C17 | −0.3 (8) | N2X—Cu2—N1X—C37X | −11.3 (13) |
| C15—C16—C17—C18 | 1.3 (8) | N2X$^{i}$—Cu2—N1X—C37X | 168.7 (13) |
| C16—C17—C18—C13 | −1.4 (7) | Cl2—Cu2—N2X—C38X | 75.9 (14) |
| P1—C13—C18—C17 | 179.4 (4) | Cl2$^{i}$—Cu2—N2X—C38X | −104.1 (14) |
| C14—C13—C18—C17 | 0.4 (7) | N1X—Cu2—N2X—C38X | −17.4 (14) |
| Cu1—P2—C19—C20 | −37.6 (4) | N1X$^{i}$—Cu2—N2X—C38X | 162.6 (14) |
| Cu1—P2—C19—C24 | 145.0 (4) | Cu2—N1X—C37X—C38X | 39 (2) |
| C25—P2—C19—C20 | 89.4 (4) | N1X—C37X—C38X—N2X | −54 (3) |
| C25—P2—C19—C24 | −88.1 (4) | N1X—C37X—C38X—C39X | −174.9 (19) |
| C31—P2—C19—C20 | −164.5 (4) | Cu2—N2X—C38X—C37X | 42 (2) |
| C31—P2—C19—C24 | 18.1 (4) | Cu2—N2X—C38X—C39X | 163.5 (14) |
| P2—C19—C20—C21 | −175.2 (4) | | |

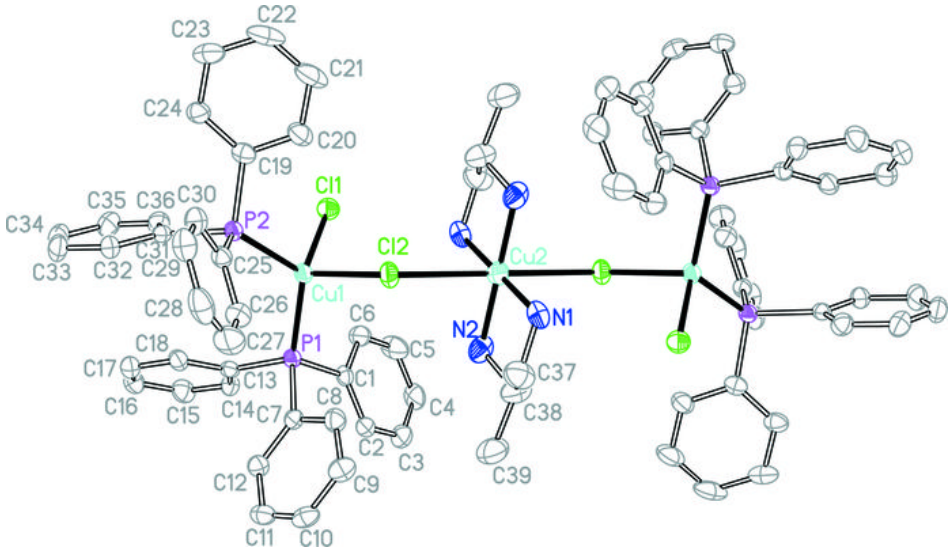
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1A···Cl1$^{i}$ | 0.92 | 2.45 | 3.330 (9) | 159 |
| N2X—H2X1···Cl1$^{i}$ | 0.92 | 2.60 | 3.495 (15) | 163 |

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

**Fig. 1**


C22
C23
C21
C24
C20
C19
Cl1
C35
C36
C30
C34
P2
Cl2
Cu2
C33
C32
C31
C29
C25
Cu1
C28
C26
C6
N2
N1
C18
C27
P1
C5
C17
C13
C1
C37
C16
C15
C14
C7
C8
C4
C38
C2
C3
C12
C9
C39
C11
C10