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Di-μ-pyridine-2-thiolato-bis[chloro(triphenylphosphine)copper(I)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 18.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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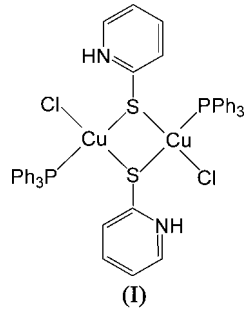
The structure of the title compound, $[Cu_2(C_5H_5NS)_2Cl_2(C_{18}H_{15}P)_2]$, shows two independent molecules, each a dimer bridged through a Cu_2S_2 rectangular plane involving the two pyridinethione S atoms and lying about a centre of symmetry. The Cu atoms have a distorted tetrahedral geometry. There is intramolecular hydrogen bonding between the pyridinium H atoms and the Cl ligands.

Comment

The dimeric title compound, $[\{CuCl(S\{C_5H_5N\})(P\{C_6H_5\}_3)\}_2]$, or $[\{CuCl(S\{C_5H_5N\})(PPh_3)\}_2]$, (I), has two half-molecules per asymmetric unit; the virtually identical molecules (I*a*) and (I*b*) each lie about a centre of symmetry (Fig. 1). At the core of each molecule there is a planar rectangular Cu_2S_2 ring, in which the Cu atoms have distorted tetrahedral geometry and the S atoms show a trigonal pyramidal arrangement. The largest difference in bond lengths between the two molecules is 0.08 Å between the bonds C332—H332 in (I*a*) and C632—H632 in (I*b*), and the largest difference in bond angles is 5° between the angles C23—N22—H22 in (I*a*) and C53—N52—H52 in (II*b*).



(I)

The monomer $[CuCl(S\{C_5H_5N\})(PPh_3)_2]$, (II) (Lobana *et al.*, 1989), has previously been reported. On forming the dimer (I), the Cu—S′ bond [where the prime (′) indicates the symmetry-related atom] is significantly longer than the Cu—S bond; 2.374 (2) Å in (II) compared with 2.3745 (5) and 2.4375 (6) Å in (I). Several complexes analogous to (I) have been reported, and comparisons are made with the Br complex $[\{CuBr(S\{C_5H_5N\})(PPh_3)\}_2]$, (III) (Karagiannidis, 1989). In (III) there is a single centrosymmetric molecule which has dimensions (and distortions from ideal values) similar to those in (I), apart from the closer equivalence of the Cu—S and Cu—S′ bonds [2.383 (1) and 2.392 (1) Å]. A third related structure, $[Cu_2(S\{C_5H_5N\})_6]Cl_2$, (IV) (Constable & Raithby, 1987), is also a dimer lying about a centre of symmetry, and has geometries in the Cu_2S_2 core plane similar to those in the Cu_2S_2 core of (I) [Cu—S_{bridge} = 2.308 (2) and

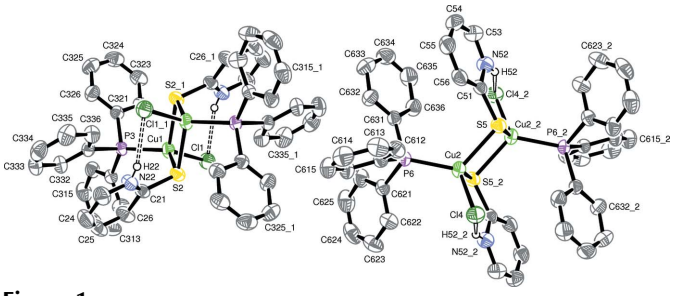


Figure 1
A view of the two independent molecules of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms, except the pyridinium H atoms, have been omitted for clarity. [Symmetry codes: (_1) $1-x, 1-y, -z$; (_2) $1-x, 1-y, 2-z$.]

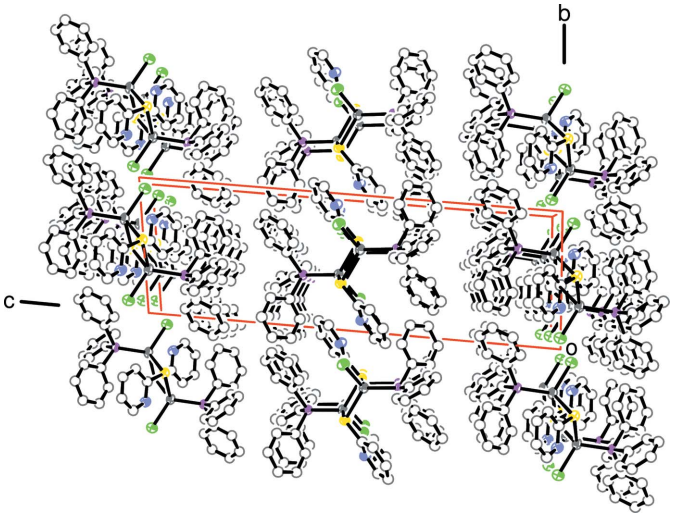


Figure 2
Packing diagram of (I), viewed along the crystallographic *a* axis. H atoms have been omitted for clarity.

2.498 (3) Å], but different geometries about the bridging S atoms [Cu—S—Cu′ = 74.3 (1)°, compared with 90.64 (2) and 91.60 (2) in (I)].

Each Cu atom in (I) is in a distorted tetrahedral geometry, the major deviations from the ideal being the S—Cu—S′/S—Cu—P angles of 89.36 (2)/121.94 (2)° and 88.40 (2)/120.99 (2)° in (I*a*) and (I*b*), respectively (see Table 1), where ′ indicates an atom related by an inversion centre. This distortion is similar to that found in (II) and (III), with that in (IV) being slightly less extreme [99.7 (1)/118.7 (1)°]. The bridging angles about the Cu atoms in (I), together with the Cu—S—Cu′ angles, show a slightly distorted rectangular Cu_2S_2 plane, which is similar to the slightly distorted square plane in (III) [S—Cu—S′ = 88.5 (1)°] but different from the parallelogram formed in (IV) [S—Cu—S′ = 105.7 (1)°].

The C_5N groups are essentially planar with the N atoms lying furthest from the mean planes at 0.007 (3) Å in both (I*a*) and (I*b*). The pyridinium H atoms in both molecules lie 0.12 (3) Å from the respective planes. The S atoms lie 0.084 (3) and 0.109 (3) Å from the planes, which are tilted with respect to the Cu_2S_2 planes; the angles between the normals to these planes are 119.55 (5) and 123.09 (5)° respectively. The CuClP planes lie at approximate right angles to the Cu_2S_2 planes, with angles between the normals to the planes of 95.22 (2) and 94.27 (2)° in the two molecules. The P atoms also have distorted tetrahedral geometries, with angles in the ranges 102.76 (8)–120.59 (6)° in (I*a*) and 102.59 (8)–120.54 (6)° in (I*b*) (see Table 1); this is similar to structures (II) and (III), where the angles lie in the ranges 99.58 (9)–119.92 (12)° and 102.4 (3)–122.5 (2)° respectively. Other bond dimensions within the ligands of (I) are as expected.

There is intramolecular hydrogen bonding between the pyridinium N—H H atoms and the Cl atoms at distances of 2.37 (3) and 2.30 (2) Å in (I*a*) and (I*b*), respectively. This is also evident in (II) and (III), with intermolecular hydrogen bonding present in (IV) between both pyridinium H atoms of the terminal S{C_5H_5N} ligands and two chloride ions (see Table 2).

In the crystal packing of (I), the (PPh_3) phenyl groups lie in layers parallel to the crystallographic *ab* plane with normal van der Waals contacts between groups in neighbouring layers, the closest being C21···C25^{iii} = 3.298 (3) Å and C51···C55^{iv} = 3.303 (3) Å [symmetry codes: (iii) $2-x, 2-y, 1-z$; (iv) $1-x, -y, 2-z$); these layers alternate with the Cu_2Cl_2(S{C_5H_5N}) layers along the crystallographic *c* axis (Fig. 2). When viewed along the crystallographic *c* axis, the molecules form columns arranged with each column surrounded by six others. This arrangement is the same as that in (III) and similar to the packing of the monomer (II), where the full (PPh_3) ligand forms layers alternating with the Cu_2Cl_2(S{C_5H_5N}) layers. It is also similar to the packing of (IV), where two (S{C_5H_5N}) ligands and the (C_5H_5N) groups of two further (S{C_5H_5N}) ligands form layers alternating with layers formed by the Cu atoms, the S atoms of two (S{C_5H_5N}) ligands and the remaining two (S{C_5H_5N}) ligands.

These results, with similarities in structure, hydrogen bonding and crystal packing between the title compound (I) and the reported structures (II), (III) and (IV), show that bond dimensions and geometries in (I) are not unusual.

Experimental

The compound SC_5H_4NH (0.2 g, 2.5 mmol) was added, under a dinitrogen atmosphere, to a suspension of PPh_3 (0.65 g, 2.5 mmol) and CuCl (0.2 g, 2.5 mmol) in CH_2Cl_2 (10 cm^3). The mixture was stirred for 2 h, then filtered. The solid was washed with CH_2Cl_2 and dried *in vacuo*. The crude product was recrystallized from EtOH over CH_2Cl_2, giving crystals of [{CuCl(S{C_5H_5N})($P(C_6H_5)_3$)}$_2$] (0.15 g 76%). IR: 1570 (*s*), 1430 (*s*), 1360 (*m*), 1125 (*s*), 1090 (*w*), 740 (*s*), 680 (*s*), 520 (*m*), 440 (*w*) cm^{-1}.

Crystal data

$[Cu_2(C_5H_5NS)_2Cl_2(C_{18}H_{15}P)_2]$
M_r = 944.84
Triclinic, $P\overline{1}$
a = 9.7076 (6) Å
b = 9.7875 (13) Å
c = 26.348 (3) Å
α = 96.918 (11)°
β = 91.942 (7)°
γ = 119.488 (8)°
V = 2150.7 (4) Å^3
Z = 2
D_x = 1.459 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 10–11°
μ = 1.32 mm^{-1}
T = 293 (2) K
Hexagonal plate, orange
0.51 × 0.33 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω/θ scans
Absorption correction: ψ scan (*EMPABS*; Sheldrick *et al.*, 1977)
T_{min} = 0.666, T_{max} = 0.709
12901 measured reflections
12512 independent reflections
9568 reflections with $I > 2\sigma(I)$
R_{int} = 0.009
θ_{max} = 30.0°
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -1 \rightarrow 37$
3 standard reflections
frequency: 167 min
intensity decay: 3.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.090
S = 1.05
12512 reflections
665 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.3413P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.3116 (6)	Cu2—Cl4	2.3127 (6)
Cu1—S2	2.3745 (5)	Cu2—S5	2.3838 (6)
Cu1—S2^{i}	2.4375 (6)	Cu2—S5^{ii}	2.4296 (5)
Cu1—P3	2.2344 (5)	Cu2—P6	2.2316 (5)
S2—C21	1.7184 (18)	S5—Cu2^{ii}	2.4296 (5)
P3—C311	1.8257 (17)	P6—C611	1.8232 (17)
P3—C321	1.8283 (17)	P6—C621	1.8269 (18)
P3—C331	1.8282 (17)	P6—C631	1.8263 (18)
P3—Cu1—Cl1	114.15 (2)	P6—Cu2—Cl4	114.24 (2)
P3—Cu1—S2	121.941 (19)	P6—Cu2—S5	120.99 (2)
Cl1—Cu1—S2	111.82 (2)	Cl4—Cu2—S5	112.23 (2)
P3—Cu1—S2^{i}	105.65 (2)	P6—Cu2—S5^{ii}	107.029 (19)
Cl1—Cu1—S2^{i}	110.26 (2)	Cl4—Cu2—S5^{ii}	110.30 (2)
S2—Cu1—S2^{i}	89.362 (19)	S5—Cu2—S5^{ii}	88.403 (19)
Cu1—S2—Cu1^{i}	90.638 (19)	Cu2—S5—Cu2^{ii}	91.598 (18)
C311—P3—C331	102.99 (8)	C611—P6—C631	102.77 (8)
C311—P3—C321	102.76 (8)	C611—P6—C621	102.59 (8)
C331—P3—C321	103.89 (8)	C631—P6—C621	104.63 (8)
C311—P3—Cu1	120.59 (6)	C611—P6—Cu2	120.54 (6)
C331—P3—Cu1	115.04 (6)	C631—P6—Cu2	113.53 (6)
C321—P3—Cu1	109.71 (6)	C621—P6—Cu2	111.10 (6)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+2$.

Table 2
Comparison of hydrogen-bond dimensions (Å, °).

Complex	N—H	N···*X*	H···*X*	N—H···*X*
(I*a*)	0.84 (3)	3.144 (2)	2.37 (3)	153 (2)
(I*b*)	0.91 (2)	3.140 (2)	2.30 (2)	154 (2)
(II)	1.01	3.079 (7)	2.22	142
(III)	0.93	3.3082 (3)	2.49	147
(IV)	1.01	3.058 (7)	2.13	151
	1.01	3.132 (8)	2.19	155

X = Cl in (I), (II) and (IV), and Br in (III).

H atoms were included initially in idealized positions, except for the N-bonded H atom, which was located in a difference electron density map, and all were subsequently refined freely [N—H = 0.84 (3) Å and C—H = 0.85 (3)–1.00 (2) Å].

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *CAD-4 Processing Program* (Hursthouse, 1976); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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References

Constable, E. C. & Raithby, P. R. (1987). *J. Chem. Soc. Dalton Trans.* pp. 2281–2283.
Enraf–Nonius (1992). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hursthouse, M. B. (1976). *CAD-4 Processing Program*. Queen Mary College, London, England.
Karagiannidis, P. (1989). *Inorg. Chim. Acta*, **156**, 47–56.
Lobana, T. S., Bhatia, P. K. & Tiekink, E. R. T. (1989). *J. Chem. Soc. Dalton Trans.* pp. 749–751.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M., Orpen, A. G., Reichert, B. E. & Raithby, P. R. (1977). *EMPABS*. 4th European Crystallographic Meeting, Oxford, Abstracts, p. 147.

supporting information

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Crystal data

$[Cu_2(C_5H_5NS)_2Cl_2(C_{18}H_{15}P)_2]$
$M_r = 944.84$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.7076$ (6) Å
$b = 9.7875$ (13) Å
$c = 26.348$ (3) Å
$\alpha = 96.918$ (11)°
$\beta = 91.942$ (7)°
$\gamma = 119.488$ (8)°
$V = 2150.7$ (4) Å^3
$Z = 2$
$F(000) = 968$
$D_x = 1.459$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 24 reflections
$\theta = 10$–11°
$\mu = 1.32$ mm^{-1}
$T = 293$ K
Hexagonal plate, orange
0.51 × 0.33 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
scintillation counter; ω/θ scans
Absorption correction: ψ scan (EMPABS; Sheldrick *et al.*, 1977)
$T_{min} = 0.666$, $T_{max} = 0.709$
12901 measured reflections
12512 independent reflections
9568 reflections with $I > 2\sigma(I)$
$R_{int} = 0.009$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.5°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -1 \rightarrow 37$
3 standard reflections every 167 min
intensity decay: 3.3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.090$
$S = 1.05$
12512 reflections
665 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.3413P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

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. Data were corrected for Lorentz-polarization effects and decay of the intensities (CAD-4 1992), absortption (Sheldrick *et al.* 1977) and negative intensities (French *et al.* 1978) before structure solution and 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.40592 (3)	0.58740 (3)	0.473401 (8)	0.04119 (6)
Cl1	0.24327 (6)	0.65210 (6)	0.52022 (2)	0.05034 (11)
S2	0.65773 (5)	0.68355 (5)	0.52030 (2)	0.03894 (9)
P3	0.38077 (5)	0.59523 (5)	0.38935 (2)	0.03279 (9)
C21	0.8034 (2)	0.7659 (2)	0.48016 (7)	0.0374 (3)
N22	0.9057 (2)	0.7115 (2)	0.47329 (7)	0.0459 (4)
H22	0.890 (3)	0.628 (3)	0.4836 (10)	0.061 (7)*
C23	1.0301 (3)	0.7729 (3)	0.44466 (10)	0.0599 (6)
H23	1.091 (3)	0.717 (4)	0.4421 (12)	0.089 (9)*
C24	1.0548 (3)	0.8949 (3)	0.42032 (9)	0.0646 (6)
H24	1.143 (3)	0.939 (3)	0.4015 (10)	0.068 (7)*
C25	0.9531 (3)	0.9549 (3)	0.42517 (9)	0.0620 (6)
H25	0.965 (3)	1.036 (3)	0.4125 (10)	0.069 (8)*
C26	0.8288 (2)	0.8928 (2)	0.45478 (9)	0.0505 (5)
H26	0.767 (3)	0.936 (3)	0.4631 (9)	0.057 (7)*
C311	0.3635 (2)	0.7561 (2)	0.36688 (6)	0.0364 (3)
C312	0.4510 (2)	0.9077 (2)	0.39528 (9)	0.0486 (4)
H312	0.509 (3)	0.923 (3)	0.4242 (9)	0.056 (7)*
C313	0.4521 (3)	1.0366 (3)	0.37759 (11)	0.0606 (6)
H313	0.509 (3)	1.132 (3)	0.3976 (9)	0.059 (7)*
C314	0.3619 (3)	1.0132 (3)	0.33228 (11)	0.0641 (6)
H314	0.360 (3)	1.099 (3)	0.3220 (11)	0.080 (8)*
C315	0.2720 (3)	0.8640 (3)	0.30486 (9)	0.0594 (6)
H315	0.213 (3)	0.847 (3)	0.2738 (11)	0.075 (8)*
C316	0.2720 (3)	0.7347 (3)	0.32167 (7)	0.0475 (4)
H316	0.215 (3)	0.629 (3)	0.3010 (9)	0.050 (6)*
C321	0.1991 (2)	0.4178 (2)	0.35821 (6)	0.0359 (3)
C322	0.0595 (2)	0.3779 (2)	0.38083 (8)	0.0429 (4)
H322	0.065 (2)	0.443 (2)	0.4128 (8)	0.044 (5)*
C323	−0.0823 (2)	0.2436 (2)	0.35970 (9)	0.0515 (5)
H323	−0.176 (3)	0.218 (3)	0.3772 (9)	0.055 (6)*
C324	−0.0849 (3)	0.1473 (3)	0.31685 (10)	0.0584 (5)
H324	−0.178 (3)	0.053 (3)	0.3020 (11)	0.078 (8)*
C325	0.0534 (3)	0.1841 (3)	0.29438 (9)	0.0612 (6)

H325	0.054 (3)	0.118 (3)	0.2651 (11)	0.076 (8)*
C326	0.1953 (3)	0.3199 (3)	0.31510 (8)	0.0491 (4)
H326	0.286 (3)	0.345 (3)	0.3000 (9)	0.059 (7)*
C331	0.5380 (2)	0.5914 (2)	0.35402 (6)	0.0363 (3)
C332	0.5990 (2)	0.6760 (3)	0.31369 (7)	0.0473 (4)
H332	0.551 (3)	0.732 (3)	0.2996 (10)	0.063 (7)*
C333	0.7241 (3)	0.6736 (3)	0.29025 (9)	0.0588 (5)
H333	0.763 (3)	0.733 (3)	0.2626 (10)	0.069 (7)*
C334	0.7889 (3)	0.5874 (3)	0.30728 (10)	0.0639 (6)
H334	0.870 (3)	0.583 (3)	0.2895 (10)	0.066 (7)*
C335	0.7288 (3)	0.5025 (3)	0.34660 (10)	0.0629 (6)
H335	0.765 (4)	0.440 (4)	0.3557 (12)	0.095 (10)*
C336	0.6045 (3)	0.5050 (3)	0.37042 (8)	0.0492 (4)
H336	0.565 (3)	0.448 (3)	0.3969 (9)	0.055 (6)*
Cu2	0.67700 (3)	0.57400 (3)	0.972730 (8)	0.04193 (6)
Cl4	0.91200 (6)	0.76884 (6)	1.02008 (2)	0.04906 (11)
S5	0.53029 (5)	0.35694 (5)	1.01763 (2)	0.03940 (9)
P6	0.69444 (5)	0.53304 (5)	0.88861 (15)	0.03279 (9)
C51	0.4583 (2)	0.1774 (2)	0.97822 (6)	0.0369 (3)
N52	0.3007 (2)	0.0718 (2)	0.97295 (6)	0.0443 (3)
H52	0.237 (3)	0.108 (3)	0.9851 (9)	0.056 (6)*
C53	0.2329 (3)	−0.0763 (3)	0.94562 (9)	0.0543 (5)
H53	0.119 (4)	−0.142 (3)	0.9440 (11)	0.084 (9)*
C54	0.3230 (3)	−0.1262 (3)	0.92092 (9)	0.0573 (5)
H54	0.275 (3)	−0.233 (3)	0.9013 (11)	0.079 (8)*
C55	0.4853 (3)	−0.0221 (3)	0.92406 (9)	0.0567 (5)
H55	0.552 (3)	−0.046 (3)	0.9081 (11)	0.077 (8)*
C56	0.5528 (3)	0.1272 (2)	0.95219 (8)	0.0470 (4)
H56	0.659 (3)	0.197 (3)	0.9552 (9)	0.054 (6)*
C611	0.86699 (19)	0.52757 (19)	0.86564 (6)	0.0354 (3)
C612	0.9391 (2)	0.4646 (2)	0.89408 (8)	0.0448 (4)
H612	0.904 (3)	0.435 (3)	0.9251 (9)	0.056 (6)*
C613	1.0626 (3)	0.4459 (3)	0.87622 (10)	0.0560 (5)
H613	1.099 (3)	0.404 (3)	0.8960 (10)	0.070 (8)*
C614	1.1174 (3)	0.4939 (3)	0.83021 (10)	0.0589 (6)
H614	1.199 (3)	0.485 (3)	0.8190 (10)	0.075 (8)*
C615	1.0508 (3)	0.5608 (3)	0.80242 (9)	0.0570 (5)
H615	1.087 (3)	0.596 (3)	0.7704 (11)	0.073 (8)*
C616	0.9258 (2)	0.5779 (2)	0.81962 (7)	0.0459 (4)
H616	0.882 (3)	0.622 (3)	0.7981 (9)	0.060 (7)*
C621	0.6913 (2)	0.6879 (2)	0.85701 (7)	0.0375 (3)
C622	0.7960 (2)	0.8450 (2)	0.87937 (9)	0.0473 (4)
H622	0.864 (3)	0.863 (3)	0.9088 (9)	0.055 (6)*
C623	0.8008 (3)	0.9692 (3)	0.85752 (11)	0.0591 (6)
H623	0.870 (3)	1.071 (3)	0.8738 (10)	0.066 (7)*
C624	0.6995 (3)	0.9369 (3)	0.81414 (11)	0.0662 (7)
H624	0.699 (3)	1.024 (4)	0.8017 (12)	0.087 (9)*
C625	0.5944 (4)	0.7833 (4)	0.79248 (10)	0.0673 (7)

H625	0.518 (3)	0.755 (3)	0.7643 (11)	0.072 (8)*
C626	0.5900 (3)	0.6573 (3)	0.81357 (8)	0.0507 (5)
H626	0.521 (3)	0.554 (3)	0.7991 (9)	0.052 (6)*
C631	0.5278 (2)	0.3475 (2)	0.85461 (6)	0.0362 (3)
C632	0.5436 (2)	0.2483 (2)	0.81579 (8)	0.0462 (4)
H632	0.638 (3)	0.284 (3)	0.8037 (9)	0.058 (7)*
C633	0.4137 (3)	0.1016 (3)	0.79546 (9)	0.0575 (5)
H633	0.429 (3)	0.037 (3)	0.7695 (10)	0.068 (7)*
C634	0.2677 (3)	0.0541 (3)	0.81331 (9)	0.0597 (6)
H634	0.178 (3)	−0.050 (3)	0.8023 (10)	0.073 (8)*
C635	0.2497 (3)	0.1526 (3)	0.85091 (9)	0.0596 (6)
H635	0.159 (3)	0.120 (3)	0.8646 (11)	0.073 (8)*
C636	0.3788 (2)	0.2982 (3)	0.87186 (8)	0.0477 (4)
H636	0.369 (3)	0.370 (3)	0.9000 (9)	0.058 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.04120 (12)	0.05046 (13)	0.03162 (11)	0.02147 (10)	0.00559 (8)	0.01180 (9)
Cl1	0.0484 (2)	0.0510 (3)	0.0555 (3)	0.0274 (2)	0.0132 (2)	0.0085 (2)
S2	0.0327 (2)	0.0374 (2)	0.0409 (2)	0.0123 (2)	0.0035 (2)	0.0105 (2)
P3	0.0346 (2)	0.0373 (2)	0.0285 (2)	0.0187 (2)	0.0041 (2)	0.0088 (2)
C21	0.0299 (7)	0.0348 (8)	0.0380 (8)	0.0085 (6)	−0.0018 (6)	0.0091 (6)
N22	0.0443 (8)	0.0412 (8)	0.0513 (9)	0.0187 (7)	0.0116 (7)	0.0151 (7)
C23	0.0526 (12)	0.0588 (13)	0.0663 (14)	0.0245 (10)	0.0220 (10)	0.0137 (11)
C24	0.0548 (13)	0.0641 (14)	0.0580 (13)	0.0139 (11)	0.0189 (11)	0.0200 (11)
C25	0.0586 (13)	0.0527 (12)	0.0565 (12)	0.0099 (10)	−0.0016 (10)	0.0303 (10)
C26	0.0410 (10)	0.0472 (10)	0.0579 (12)	0.0155 (8)	−0.0039 (8)	0.0219 (9)
C311	0.0376 (8)	0.0400 (8)	0.0364 (8)	0.0215 (7)	0.0088 (6)	0.0114 (6)
C312	0.0422 (10)	0.0469 (10)	0.0574 (12)	0.0239 (8)	0.0002 (9)	0.0051 (9)
C313	0.0539 (12)	0.0386 (10)	0.0900 (18)	0.0228 (9)	0.0133 (12)	0.0120 (11)
C314	0.0699 (15)	0.0595 (13)	0.0852 (17)	0.0418 (12)	0.0291 (13)	0.0399 (13)
C315	0.0739 (15)	0.0739 (15)	0.0522 (12)	0.0484 (13)	0.0131 (11)	0.0311 (11)
C316	0.0585 (11)	0.0528 (11)	0.0384 (9)	0.0318 (9)	0.0049 (8)	0.0137 (8)
C321	0.0378 (8)	0.0371 (8)	0.0351 (8)	0.0196 (7)	0.0016 (6)	0.0096 (6)
C322	0.0420 (9)	0.0407 (9)	0.0490 (10)	0.0224 (8)	0.0067 (8)	0.0090 (8)
C323	0.0385 (9)	0.0491 (11)	0.0655 (13)	0.0194 (8)	0.0035 (9)	0.0166 (9)
C324	0.0482 (11)	0.0468 (11)	0.0647 (14)	0.0137 (9)	−0.0124 (10)	0.0058 (10)
C325	0.0636 (14)	0.0563 (12)	0.0500 (12)	0.0242 (11)	−0.0082 (10)	−0.0089 (10)
C326	0.0482 (10)	0.0541 (11)	0.0407 (10)	0.0239 (9)	0.0023 (8)	0.0010 (8)
C331	0.0358 (8)	0.0418 (8)	0.0314 (7)	0.0199 (7)	0.0023 (6)	0.0048 (6)
C332	0.0494 (10)	0.0570 (11)	0.0413 (9)	0.0289 (9)	0.0135 (8)	0.0153 (8)
C333	0.0577 (13)	0.0716 (14)	0.0503 (12)	0.0325 (11)	0.0224 (10)	0.0153 (10)
C334	0.0509 (12)	0.0798 (16)	0.0626 (14)	0.0367 (12)	0.0148 (10)	−0.0047 (12)
C335	0.0637 (14)	0.0808 (16)	0.0644 (14)	0.0525 (13)	0.0078 (11)	0.0062 (12)
C336	0.0534 (11)	0.0577 (11)	0.0486 (11)	0.0357 (10)	0.0087 (9)	0.0131 (9)
Cu2	0.04974 (13)	0.04424 (12)	0.03210 (11)	0.02372 (10)	0.00784 (9)	0.00510 (8)
Cl4	0.0427 (2)	0.0490 (2)	0.0527 (3)	0.0216 (2)	0.00076 (19)	0.0057 (2)

S5	0.0467 (2)	0.0353 (2)	0.0420 (2)	0.0237 (2)	0.0100 (2)	0.0103 (2)
P6	0.0348 (2)	0.0365 (2)	0.0288 (2)	0.0189 (2)	0.0054 (2)	0.0056 (2)
C51	0.0466 (9)	0.0357 (8)	0.0374 (8)	0.0248 (7)	0.0124 (7)	0.0156 (6)
N52	0.0447 (8)	0.0421 (8)	0.0515 (9)	0.0255 (7)	0.0099 (7)	0.0080 (7)
C53	0.0540 (12)	0.0438 (10)	0.0610 (13)	0.0224 (9)	0.0017 (10)	0.0050 (9)
C54	0.0787 (15)	0.0453 (11)	0.0521 (12)	0.0352 (11)	0.0066 (11)	0.0025 (9)
C55	0.0817 (16)	0.0585 (12)	0.0524 (11)	0.0491 (12)	0.0303 (11)	0.0163 (9)
C56	0.0527 (11)	0.0452 (10)	0.0529 (11)	0.0284 (9)	0.0238 (9)	0.0185 (8)
C611	0.0343 (8)	0.0362 (8)	0.0366 (8)	0.0184 (7)	0.0053 (6)	0.0043 (6)
C612	0.0414 (9)	0.0450 (10)	0.0490 (10)	0.0211 (8)	0.0045 (8)	0.0140 (8)
C613	0.0475 (11)	0.0542 (12)	0.0771 (15)	0.0331 (10)	0.0034 (10)	0.0132 (11)
C614	0.0472 (11)	0.0621 (13)	0.0746 (15)	0.0341 (10)	0.0154 (10)	0.0026 (11)
C615	0.0577 (12)	0.0675 (13)	0.0517 (12)	0.0350 (11)	0.0218 (10)	0.0085 (10)
C616	0.0515 (10)	0.0575 (11)	0.0389 (9)	0.0337 (9)	0.0120 (8)	0.0115 (8)
C621	0.0370 (8)	0.0450 (9)	0.0390 (8)	0.0254 (7)	0.0115 (7)	0.0123 (7)
C622	0.0413 (9)	0.0459 (10)	0.0609 (12)	0.0249 (8)	0.0090 (9)	0.0144 (9)
C623	0.0546 (12)	0.0464 (11)	0.0873 (17)	0.0291 (10)	0.0265 (12)	0.0264 (11)
C624	0.0823 (17)	0.0750 (16)	0.0742 (16)	0.0557 (14)	0.0362 (13)	0.0438 (13)
C625	0.0850 (17)	0.0925 (19)	0.0524 (13)	0.0616 (16)	0.0102 (12)	0.0295 (13)
C626	0.0591 (12)	0.0599 (12)	0.0401 (10)	0.0345 (10)	0.0029 (9)	0.0113 (9)
C631	0.0364 (8)	0.0388 (8)	0.0327 (8)	0.0177 (7)	0.0036 (6)	0.0080 (6)
C632	0.0443 (10)	0.0478 (10)	0.0421 (9)	0.0212 (8)	0.0030 (8)	0.0001 (8)
C633	0.0623 (13)	0.0506 (11)	0.0528 (12)	0.0275 (10)	−0.0076 (10)	−0.0087 (9)
C634	0.0510 (12)	0.0475 (11)	0.0576 (13)	0.0085 (9)	−0.0103 (10)	0.0067 (9)
C635	0.0367 (10)	0.0699 (14)	0.0548 (12)	0.0131 (10)	0.0015 (9)	0.0126 (11)
C636	0.0396 (9)	0.0554 (11)	0.0429 (10)	0.0203 (8)	0.0060 (7)	0.0052 (8)

Geometric parameters (Å, º)

Cu1—Cl1	2.3116 (6)	Cu2—Cl4	2.3127 (6)
Cu1—S2	2.3745 (5)	Cu2—S5	2.3838 (6)
Cu1—S2^{i}	2.4375 (6)	Cu2—S5^{ii}	2.4296 (5)
Cu1—P3	2.2344 (5)	Cu2—P6	2.2316 (5)
S2—Cu1^{i}	2.4376 (6)	S5—C51	1.7194 (18)
S2—C21	1.7184 (18)	S5—Cu2^{ii}	2.4296 (5)
P3—C311	1.8257 (17)	P6—C611	1.8232 (17)
P3—C321	1.8283 (17)	P6—C621	1.8269 (18)
P3—C331	1.8282 (17)	P6—C631	1.8263 (18)
C21—N22	1.346 (2)	C51—N52	1.350 (2)
C21—C26	1.400 (3)	C51—C56	1.399 (3)
N22—C23	1.359 (3)	N52—C53	1.353 (3)
N22—H22	0.84 (3)	N52—H52	0.91 (2)
C23—C24	1.344 (4)	C53—C54	1.346 (3)
C23—H23	0.98 (3)	C53—H53	0.97 (3)
C24—C25	1.377 (4)	C54—C55	1.384 (4)
C24—H24	0.94 (3)	C54—H54	0.98 (3)
C25—C26	1.375 (3)	C55—C56	1.370 (3)
C25—H25	0.85 (3)	C55—H55	0.89 (3)

C26—H26	0.90 (2)	C56—H56	0.91 (2)
C311—C312	1.390 (3)	C611—C612	1.389 (3)
C311—C316	1.392 (3)	C611—C616	1.397 (2)
C312—C313	1.392 (3)	C612—C613	1.389 (3)
C312—H312	0.89 (2)	C612—H612	0.92 (2)
C313—C314	1.382 (4)	C613—C614	1.381 (4)
C313—H313	0.90 (2)	C613—H613	0.87 (3)
C314—C315	1.365 (4)	C614—C615	1.372 (4)
C314—H314	0.92 (3)	C614—H614	0.90 (3)
C315—C316	1.389 (3)	C615—C616	1.387 (3)
C315—H315	0.93 (3)	C615—H615	0.96 (3)
C316—H316	0.97 (2)	C616—H616	0.95 (3)
C321—C326	1.382 (3)	C621—C626	1.385 (3)
C321—C322	1.391 (2)	C621—C622	1.396 (3)
C322—C323	1.387 (3)	C622—C623	1.387 (3)
C322—H322	0.98 (2)	C622—H622	0.94 (2)
C323—C324	1.372 (3)	C623—C624	1.380 (4)
C323—H323	0.97 (2)	C623—H623	0.92 (3)
C324—C325	1.383 (4)	C624—C625	1.367 (4)
C324—H324	0.94 (3)	C624—H624	0.95 (3)
C325—C326	1.390 (3)	C625—C626	1.395 (3)
C325—H325	0.95 (3)	C625—H625	0.94 (3)
C326—H326	0.91 (2)	C626—H626	0.91 (2)
C331—C336	1.386 (3)	C631—C632	1.390 (3)
C331—C332	1.392 (2)	C631—C636	1.393 (2)
C332—C333	1.390 (3)	C632—C633	1.387 (3)
C332—H332	0.97 (3)	C632—H632	0.89 (2)
C333—C334	1.380 (4)	C633—C634	1.377 (3)
C333—H333	0.95 (3)	C633—H633	0.94 (3)
C334—C335	1.369 (4)	C634—C635	1.374 (4)
C334—H334	0.94 (3)	C634—H634	0.96 (3)
C335—C336	1.389 (3)	C635—C636	1.383 (3)
C335—H335	0.89 (3)	C635—H635	0.88 (3)
C336—H336	0.92 (2)	C636—H636	1.00 (2)

P3—Cu1—Cl1	114.15 (2)	P6—Cu2—Cl4	114.24 (2)
P3—Cu1—S2	121.941 (19)	P6—Cu2—S5	120.99 (2)
Cl1—Cu1—S2	111.82 (2)	Cl4—Cu2—S5	112.23 (2)
P3—Cu1—S2^{i}	105.65 (2)	P6—Cu2—S5^{ii}	107.029 (19)
Cl1—Cu1—S2^{i}	110.26 (2)	Cl4—Cu2—S5^{ii}	110.30 (2)
S2—Cu1—S2^{i}	89.362 (19)	S5—Cu2—S5^{ii}	88.403 (19)
C21—S2—Cu1	108.75 (6)	C51—S5—Cu2	111.47 (6)
C21—S2—Cu1^{i}	110.70 (7)	C51—S5—Cu2^{ii}	110.75 (6)
Cu1—S2—Cu1^{i}	90.638 (19)	Cu2—S5—Cu2^{ii}	91.598 (18)
C311—P3—C331	102.99 (8)	C611—P6—C631	102.77 (8)
C311—P3—C321	102.76 (8)	C611—P6—C621	102.59 (8)
C331—P3—C321	103.89 (8)	C631—P6—C621	104.63 (8)
C311—P3—Cu1	120.59 (6)	C611—P6—Cu2	120.54 (6)

C331—P3—Cu1	115.04 (6)	C631—P6—Cu2	113.53 (6)
C321—P3—Cu1	109.71 (6)	C621—P6—Cu2	111.10 (6)
N22—C21—C26	116.15 (17)	N52—C51—C56	116.00 (17)
N22—C21—S2	119.43 (13)	N52—C51—S5	119.27 (13)
C26—C21—S2	124.38 (16)	C56—C51—S5	124.67 (15)
C21—N22—C23	124.51 (19)	C51—N52—C53	124.13 (18)
C21—N22—H22	121.6 (18)	C51—N52—H52	116.8 (15)
C23—N22—H22	113.5 (18)	C53—N52—H52	118.5 (16)
C24—C23—N22	119.5 (2)	C54—C53—N52	120.3 (2)
C24—C23—H23	125.6 (18)	C54—C53—H53	122.2 (18)
N22—C23—H23	114.8 (18)	N52—C53—H53	117.5 (18)
C23—C24—C25	119.0 (2)	C53—C54—C55	118.3 (2)
C23—C24—H24	118.8 (17)	C53—C54—H54	120.9 (17)
C25—C24—H24	122.2 (16)	C55—C54—H54	120.8 (17)
C26—C25—C24	121.0 (2)	C56—C55—C54	120.9 (2)
C26—C25—H25	115.0 (18)	C56—C55—H55	115.8 (19)
C24—C25—H25	123.9 (18)	C54—C55—H55	123.3 (19)
C25—C26—C21	119.9 (2)	C55—C56—C51	120.4 (2)
C25—C26—H26	124.9 (16)	C55—C56—H56	122.4 (15)
C21—C26—H26	114.7 (16)	C51—C56—H56	117.2 (15)
C312—C311—C316	118.74 (17)	C612—C611—C616	118.57 (17)
C312—C311—P3	118.23 (14)	C612—C611—P6	118.52 (14)
C316—C311—P3	122.98 (14)	C616—C611—P6	122.85 (14)
C313—C312—C311	120.4 (2)	C613—C612—C611	120.83 (19)
C313—C312—H312	119.9 (15)	C613—C612—H612	119.6 (15)
C311—C312—H312	119.6 (15)	C611—C612—H612	119.6 (15)
C314—C313—C312	119.9 (2)	C614—C613—C612	119.7 (2)
C314—C313—H313	122.9 (16)	C614—C613—H613	125.6 (18)
C312—C313—H313	117.1 (16)	C612—C613—H613	114.7 (18)
C315—C314—C313	120.1 (2)	C615—C614—C613	120.2 (2)
C315—C314—H314	121.2 (18)	C615—C614—H614	119.7 (18)
C313—C314—H314	118.7 (18)	C613—C614—H614	120.0 (18)
C314—C315—C316	120.6 (2)	C614—C615—C616	120.5 (2)
C314—C315—H315	120.7 (17)	C614—C615—H615	122.1 (17)
C316—C315—H315	118.6 (17)	C616—C615—H615	117.4 (16)
C315—C316—C311	120.2 (2)	C615—C616—C611	120.19 (19)
C315—C316—H316	121.0 (13)	C615—C616—H616	116.6 (15)
C311—C316—H316	118.6 (13)	C611—C616—H616	123.2 (15)
C326—C321—C322	119.10 (17)	C626—C621—C622	119.31 (18)
C326—C321—P3	123.55 (14)	C626—C621—P6	123.84 (15)
C322—C321—P3	117.30 (13)	C622—C621—P6	116.83 (14)
C323—C322—C321	120.43 (19)	C623—C622—C621	120.2 (2)
C323—C322—H322	121.0 (12)	C623—C622—H622	121.8 (15)
C321—C322—H322	118.5 (12)	C621—C622—H622	117.9 (14)
C324—C323—C322	120.0 (2)	C624—C623—C622	119.8 (2)
C324—C323—H323	121.9 (14)	C624—C623—H623	122.5 (17)
C322—C323—H323	117.9 (14)	C622—C623—H623	117.6 (17)
C323—C324—C325	120.2 (2)	C625—C624—C623	120.5 (2)

C323—C324—H324	122.7 (17)	C625—C624—H624	121.3 (19)
C325—C324—H324	117.1 (17)	C623—C624—H624	118.0 (19)
C324—C325—C326	119.8 (2)	C624—C625—C626	120.3 (2)
C324—C325—H325	121.4 (17)	C624—C625—H625	123.5 (17)
C326—C325—H325	118.8 (17)	C626—C625—H625	116.0 (17)
C321—C326—C325	120.4 (2)	C621—C626—C625	119.9 (2)
C321—C326—H326	119.8 (15)	C621—C626—H626	119.3 (15)
C325—C326—H326	119.8 (15)	C625—C626—H626	120.8 (15)
C336—C331—C332	118.82 (17)	C632—C631—C636	118.80 (17)
C336—C331—P3	117.40 (14)	C632—C631—P6	123.90 (14)
C332—C331—P3	123.70 (14)	C636—C631—P6	117.11 (14)
C333—C332—C331	120.5 (2)	C633—C632—C631	120.3 (2)
C333—C332—H332	118.2 (15)	C633—C632—H632	121.6 (15)
C331—C332—H332	121.2 (15)	C631—C632—H632	118.0 (16)
C334—C333—C332	119.8 (2)	C634—C633—C632	120.1 (2)
C334—C333—H333	121.9 (16)	C634—C633—H633	121.9 (17)
C332—C333—H333	118.4 (16)	C632—C633—H633	118.0 (17)
C335—C334—C333	120.2 (2)	C635—C634—C633	120.1 (2)
C335—C334—H334	121.6 (16)	C635—C634—H634	117.4 (16)
C333—C334—H334	118.1 (16)	C633—C634—H634	122.3 (16)
C334—C335—C336	120.4 (2)	C634—C635—C636	120.2 (2)
C334—C335—H335	120 (2)	C634—C635—H635	120.9 (18)
C336—C335—H335	119 (2)	C636—C635—H635	118.5 (18)
C331—C336—C335	120.3 (2)	C635—C636—C631	120.4 (2)
C331—C336—H336	120.2 (15)	C635—C636—H636	121.3 (14)
C335—C336—H336	119.4 (15)	C631—C636—H636	118.3 (14)

P3—Cu1—S2—C21	4.03 (7)	P6—Cu2—S5—C51	4.10 (7)
Cl1—Cu1—S2—C21	−136.22 (7)	Cl4—Cu2—S5—C51	−135.62 (7)
S2^{i}—Cu1—S2—C21	112.15 (7)	S5^{ii}—Cu2—S5—C51	113.07 (7)
P3—Cu1—S2—Cu1^{i}	−108.12 (2)	P6—Cu2—S5—Cu2^{ii}	−108.97 (2)
Cl1—Cu1—S2—Cu1^{i}	111.63 (2)	Cl4—Cu2—S5—Cu2^{ii}	111.31 (2)
S2^{i}—Cu1—S2—Cu1^{i}	0.0	S5^{ii}—Cu2—S5—Cu2^{ii}	0.0
Cl1—Cu1—P3—C311	41.80 (7)	Cl4—Cu2—P6—C611	42.17 (7)
S2—Cu1—P3—C311	−97.62 (7)	S5—Cu2—P6—C611	−96.80 (7)
S2^{i}—Cu1—P3—C311	163.12 (7)	S5^{ii}—Cu2—P6—C611	164.57 (6)
Cl1—Cu1—P3—C331	166.17 (6)	Cl4—Cu2—P6—C631	164.64 (6)
S2—Cu1—P3—C331	26.75 (7)	S5—Cu2—P6—C631	25.66 (7)
S2^{i}—Cu1—P3—C331	−72.52 (6)	S5^{ii}—Cu2—P6—C631	−72.97 (6)
Cl1—Cu1—P3—C321	−77.17 (6)	Cl4—Cu2—P6—C621	−77.76 (6)
S2—Cu1—P3—C321	143.41 (6)	S5—Cu2—P6—C621	143.27 (6)
S2^{i}—Cu1—P3—C321	44.14 (6)	S5^{ii}—Cu2—P6—C621	44.64 (6)
Cu1—S2—C21—N22	−123.41 (13)	Cu2—S5—C51—N52	−124.42 (13)
Cu1^{i}—S2—C21—N22	−25.32 (16)	Cu2^{ii}—S5—C51—N52	−23.99 (15)
Cu1—S2—C21—C26	59.17 (17)	Cu2—S5—C51—C56	58.62 (17)
Cu1^{i}—S2—C21—C26	157.27 (15)	Cu2^{ii}—S5—C51—C56	159.05 (14)
C26—C21—N22—C23	1.2 (3)	C56—C51—N52—C53	1.6 (3)
S2—C21—N22—C23	−176.46 (17)	S5—C51—N52—C53	−175.66 (16)

C21—N22—C23—C24	−1.1 (4)	C51—N52—C53—C54	−0.9 (3)
N22—C23—C24—C25	0.1 (4)	N52—C53—C54—C55	−0.4 (3)
C23—C24—C25—C26	0.7 (4)	C53—C54—C55—C56	0.9 (3)
C24—C25—C26—C21	−0.6 (3)	C54—C55—C56—C51	−0.2 (3)
N22—C21—C26—C25	−0.3 (3)	N52—C51—C56—C55	−1.0 (3)
S2—C21—C26—C25	177.17 (17)	S5—C51—C56—C55	176.05 (16)
C331—P3—C311—C312	−93.35 (15)	C631—P6—C611—C612	−93.21 (15)
C321—P3—C311—C312	158.90 (15)	C621—P6—C611—C612	158.36 (15)
Cu1—P3—C311—C312	36.51 (17)	Cu2—P6—C611—C612	34.31 (17)
C331—P3—C311—C316	84.04 (16)	C631—P6—C611—C616	84.08 (17)
C321—P3—C311—C316	−23.71 (17)	C621—P6—C611—C616	−24.35 (17)
Cu1—P3—C311—C316	−146.09 (14)	Cu2—P6—C611—C616	−148.40 (14)
C316—C311—C312—C313	−2.7 (3)	C616—C611—C612—C613	−2.6 (3)
P3—C311—C312—C313	174.78 (17)	P6—C611—C612—C613	174.78 (16)
C311—C312—C313—C314	2.0 (3)	C611—C612—C613—C614	1.6 (3)
C312—C313—C314—C315	−0.1 (4)	C612—C613—C614—C615	0.4 (4)
C313—C314—C315—C316	−1.0 (4)	C613—C614—C615—C616	−1.3 (4)
C314—C315—C316—C311	0.2 (3)	C614—C615—C616—C611	0.3 (3)
C312—C311—C316—C315	1.7 (3)	C612—C611—C616—C615	1.7 (3)
P3—C311—C316—C315	−175.71 (16)	P6—C611—C616—C615	−175.62 (17)
C311—P3—C321—C326	102.17 (17)	C611—P6—C621—C626	101.18 (17)
C331—P3—C321—C326	−4.89 (18)	C631—P6—C621—C626	−5.82 (18)
Cu1—P3—C321—C326	−128.38 (15)	Cu2—P6—C621—C626	−128.72 (15)
C311—P3—C321—C322	−80.35 (15)	C611—P6—C621—C622	−80.27 (15)
C331—P3—C321—C322	172.59 (13)	C631—P6—C621—C622	172.73 (14)
Cu1—P3—C321—C322	49.10 (14)	Cu2—P6—C621—C622	49.83 (15)
C326—C321—C322—C323	−1.5 (3)	C626—C621—C622—C623	−1.5 (3)
P3—C321—C322—C323	−179.11 (15)	P6—C621—C622—C623	179.84 (16)
C321—C322—C323—C324	1.4 (3)	C621—C622—C623—C624	1.3 (3)
C322—C323—C324—C325	−0.4 (3)	C622—C623—C624—C625	−0.1 (4)
C323—C324—C325—C326	−0.5 (4)	C623—C624—C625—C626	−0.9 (4)
C322—C321—C326—C325	0.6 (3)	C622—C621—C626—C625	0.6 (3)
P3—C321—C326—C325	178.04 (17)	P6—C621—C626—C625	179.07 (17)
C324—C325—C326—C321	0.4 (4)	C624—C625—C626—C621	0.7 (4)
C311—P3—C331—C336	166.35 (15)	C611—P6—C631—C632	−8.33 (18)
C321—P3—C331—C336	−86.75 (16)	C621—P6—C631—C632	98.54 (17)
Cu1—P3—C331—C336	33.18 (17)	Cu2—P6—C631—C632	−140.16 (15)
C311—P3—C331—C332	−10.35 (18)	C611—P6—C631—C636	166.48 (15)
C321—P3—C331—C332	96.54 (17)	C621—P6—C631—C636	−86.65 (16)
Cu1—P3—C331—C332	−143.53 (14)	Cu2—P6—C631—C636	34.65 (16)
C336—C331—C332—C333	0.1 (3)	C636—C631—C632—C633	−1.3 (3)
P3—C331—C332—C333	176.79 (17)	P6—C631—C632—C633	173.43 (17)
C331—C332—C333—C334	−0.4 (3)	C631—C632—C633—C634	0.6 (3)
C332—C333—C334—C335	1.0 (4)	C632—C633—C634—C635	0.8 (4)
C333—C334—C335—C336	−1.4 (4)	C633—C634—C635—C636	−1.5 (4)
C332—C331—C336—C335	−0.5 (3)	C634—C635—C636—C631	0.8 (3)

P3—C331—C336—C335	−177.38 (18)	C632—C631—C636—C635	0.5 (3)
C334—C335—C336—C331	1.1 (4)	P6—C631—C636—C635	−174.53 (17)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N22—H22···Cl1^{i}	0.84 (3)	2.37 (3)	3.1436 (18)	153 (2)
N52—H52···Cl4^{ii}	0.91 (2)	2.30 (2)	3.1398 (17)	154 (2)

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