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(Pyrimidine-2-thiolato-κ^2N,S)bis(triphenylphosphine-κP)copper(I)

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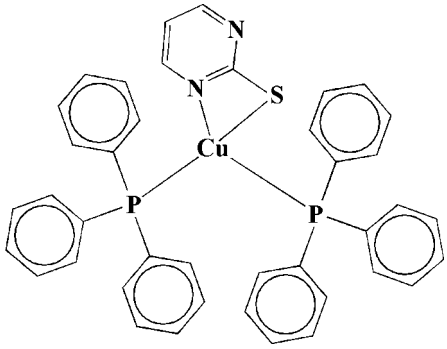
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.113; data-to-parameter ratio = 17.4.

The pyrimidine-2-thiolate ligand in the title copper(I) complex, $[Cu(C_4H_3N_2S)(C_{18}H_{15}P)_2]$, chelates the metal atom through the exocyclic S atom and one heterocyclic N atom. Two triphenylphosphine ligands complete the approximately tetrahedral coordination geometry about the Cu^I atom. In the crystal structure, intermolecular C—H···S hydrogen bonds connect the mononuclear complexes into a two-dimensional network.

Related literature

For general background, see: Krebs & Henkel (1991). For details of metal complexes of pyrimidine-2-thiolate, see: Cookson & Tiekink (1993); Cotton & Ilsley (1982); Su *et al.* (1999); Yap & Jensen (1992); Zhao *et al.* (2001). For details of the related thiones, see Karagiannidis *et al.* (1990); Lecomte *et al.* (1989). For a related structure, see: Li *et al.* (2004).



Experimental

Crystal data

$[Cu(C_4H_3N_2S)(C_{18}H_{15}P)_2]$
M_r = 699.22
Triclinic, $P\overline{1}$
a = 9.3092 (6) Å
b = 11.0636 (7) Å
c = 18.8384 (12) Å
α = 93.181 (1)°
β = 91.912 (2)°
γ = 113.810 (2)°
V = 1769.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 295 (2) K
0.28 × 0.25 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.808, T_{max} = 0.857
14456 measured reflections
7227 independent reflections
5598 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.113
S = 1.01
7227 reflections
415 parameters
102 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···S1	0.93	2.83	3.661 (3)	150
C13—H13···S1^{i}	0.93	2.73	3.613 (4)	159

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); 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: SJ2336).

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supplementary materials

Acta Cryst. (2007). E**63**, m2412 [**doi:10.1107/S1600536807040925**]

(Pyrimidine-2-thiolato-κ^2N,S)bis(triphenylphosphine-κP)copper(I)

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Comment

Heterocyclic thiones have attracted much attention as ligands in metal complexes because of their relevance in biological systems (Krebs & Henkel, 1991). Pyrimidine-2-thione and the corresponding thiolate can adopt different coordination modes to yield a variety of coordination complexes (Cookson & Tiekink, 1993; Cotton & Ilsley, 1982; Karagiannidis *et al.*, 1990; Lecomte *et al.*, 1989; Su *et al.*, 1999; Yap & Jensen, 1992; Zhao *et al.*, 2001).

In the earlier study on the complex of copper(I) ion with both phosphine and a heterocyclic mercaptan, Li *et al.* have found that the heterocyclic thione ligands exist in the thione form in the adduct, the ligands coordinate in a monodentate fashion through the doubly bonded S atom (Li *et al.*, 2004). In this work, the deprotonated ligand coordinates to the copper(I) ion in a chelate manner through an endocyclic N atom and the exocyclic S atom, giving the title complex (Fig. 1). The Cu atom exists in a tetrahedral environment.

A two-dimensional supramolecular network (Fig. 2) is formed by the intermolecular C—H···S hydrogen bonds [H···S 2.73 (3), 2.83 (2) Å; C—H···S 158.6 (1), 149.6 (1) °].

Experimental

Sodium pyrimidine-2-thiolate was prepared through the reaction of pyrimidine-2-thione with sodium metal in dry tetrahydrofuran. To a stirred solution of $Cu(NO_3)_2{\cdot}3H_2O$ (60.9 mg, 0.25 mmol) in methanol (5 ml) was added a methanol solution (5 ml) of sodium pyrimidine-2-thiolate (34.0 mg, 0.25 mmol) and a precipitate formed immediately. The resulting brown powder was added to a stirred solution of triphenylphosphine (130.2 mg, 0.5 mmol) in acetone (7 ml), forming a clear yellow solution. This was left standing at room temperature. Colorless block-shaped crystals of the title compound were obtained after two months. Yield: 55.6 mg (32%).

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, U_{iso} = 1.2U_{eq}(C) for aromatic H-atoms.

Figures

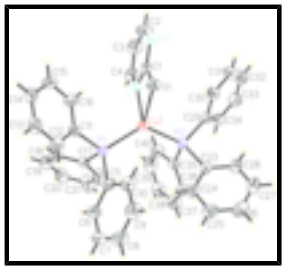


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level, and H atoms as spheres of arbitrary radius.

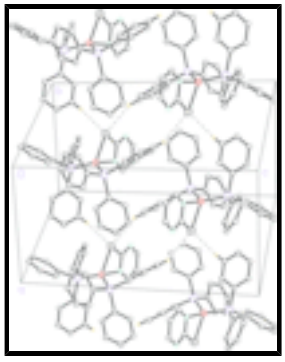


Fig. 2. Packing diagram showing the C—H···S hydrogen bonding interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

(Pyrimidine-2-thiolato-κ^2*N*,*S*)bis(triphenylphosphine- κ*P*)copper(I)

Crystal data

$[Cu(C_4H_3N_2S)(C_{18}H_{15}P)_2]$	$Z = 2$
$M_r = 699.22$	$F_{000} = 724$
Triclinic, $P\overline{1}$	$D_x = 1.313$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.3092$ (6) Å	Cell parameters from 3662 reflections
$b = 11.0636$ (7) Å	$\theta = 2.2$–23.3º
$c = 18.8384$ (12) Å	$\mu = 0.80$ mm^{-1}
$\alpha = 93.181$ (1)º	$T = 295$ (2) K
$\beta = 91.912$ (2)º	Block, colourless
$\gamma = 113.810$ (2)º	0.28 × 0.25 × 0.20 mm
$V = 1769.1$ (2) Å^3	

Data collection

Bruker APEX area-detector diffractometer	7227 independent reflections
Radiation source: fine-focus sealed tube	5598 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 295$(2) K	$\theta_{max} = 26.5$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan	$h = -11 \rightarrow 11$

(SADABS; Sheldrick, 1996)
T_{min} = 0.808, T_{max} = 0.857
14456 measured reflections
k = −13→13
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.113
S = 1.01
7227 reflections
415 parameters
102 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.2219P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: none

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}
Cu1	0.69666 (4)	0.54945 (3)	0.719137 (16)	0.04441 (12)
S1	0.86486 (8)	0.44086 (7)	0.68664 (4)	0.0569 (2)
P1	0.63061 (8)	0.52595 (7)	0.83325 (4)	0.04319 (17)
P2	0.73004 (8)	0.72462 (6)	0.65674 (4)	0.04140 (17)
N1	0.5631 (3)	0.3595 (2)	0.66490 (11)	0.0485 (5)
N2	0.6660 (4)	0.1983 (3)	0.63669 (15)	0.0736 (8)
C1	0.6832 (3)	0.3203 (3)	0.65968 (13)	0.0487 (6)
C2	0.4191 (4)	0.2706 (3)	0.64506 (17)	0.0679 (8)
H2	0.3348	0.2951	0.6477	0.082*
C3	0.3917 (5)	0.1435 (4)	0.6207 (2)	0.0885 (12)
H3	0.2912	0.0809	0.6067	0.106*
C4	0.5206 (6)	0.1146 (4)	0.6183 (2)	0.0921 (12)
H4	0.5046	0.0287	0.6024	0.110*
C5	0.5714 (3)	0.3579 (3)	0.86245 (14)	0.0492 (6)

C6	0.6564 (4)	0.2863 (3)	0.84107 (17)	0.0695 (9)
H6	0.7418	0.3244	0.8133	0.083*
C7	0.6150 (6)	0.1576 (4)	0.8607 (2)	0.0943 (12)
H7	0.6732	0.1099	0.8468	0.113*
C8	0.4865 (6)	0.1014 (4)	0.9011 (2)	0.0940 (13)
H8	0.4569	0.0149	0.9136	0.113*
C9	0.4043 (5)	0.1710 (3)	0.92248 (19)	0.0798 (10)
H9	0.3194	0.1328	0.9505	0.096*
C10	0.4445 (4)	0.2988 (3)	0.90314 (16)	0.0622 (8)
H10	0.3855	0.3453	0.9177	0.075*
C11	0.4607 (3)	0.5631 (3)	0.85071 (14)	0.0463 (6)
C12	0.3271 (3)	0.4996 (3)	0.80554 (18)	0.0672 (8)
H12	0.3264	0.4394	0.7689	0.081*
C13	0.1948 (4)	0.5252 (4)	0.8146 (2)	0.0862 (11)
H13	0.1045	0.4798	0.7851	0.103*
C14	0.1963 (4)	0.6172 (4)	0.8668 (2)	0.0851 (11)
H14	0.1083	0.6362	0.8719	0.102*
C15	0.3260 (4)	0.6802 (4)	0.9110 (2)	0.0783 (10)
H15	0.3267	0.7419	0.9468	0.094*
C16	0.4579 (3)	0.6535 (3)	0.90348 (16)	0.0588 (7)
H16	0.5461	0.6972	0.9345	0.071*
C17	0.7791 (3)	0.6296 (3)	0.90186 (14)	0.0457 (6)
C18	0.8176 (3)	0.5834 (3)	0.96336 (15)	0.0600 (7)
H18	0.7650	0.4946	0.9719	0.072*
C19	0.9331 (4)	0.6677 (4)	1.01194 (18)	0.0782 (10)
H19	0.9580	0.6352	1.0529	0.094*
C20	1.0117 (4)	0.7987 (4)	1.0007 (2)	0.0820 (11)
H20	1.0899	0.8552	1.0336	0.098*
C21	0.9738 (4)	0.8456 (3)	0.9405 (2)	0.0796 (10)
H21	1.0260	0.9348	0.9328	0.095*
C22	0.8588 (3)	0.7619 (3)	0.89089 (16)	0.0610 (8)
H22	0.8350	0.7951	0.8499	0.073*
C23	0.8644 (3)	0.8830 (2)	0.70027 (14)	0.0453 (6)
C24	1.0025 (3)	0.8879 (3)	0.73323 (17)	0.0609 (8)
H24	1.0219	0.8116	0.7327	0.073*
C25	1.1113 (4)	1.0045 (4)	0.7668 (2)	0.0801 (10)
H25	1.2046	1.0071	0.7876	0.096*
C26	1.0822 (5)	1.1159 (4)	0.7695 (2)	0.0862 (11)
H26	1.1542	1.1937	0.7935	0.103*
C27	0.9471 (5)	1.1137 (3)	0.7370 (2)	0.0795 (10)
H27	0.9285	1.1903	0.7383	0.095*
C28	0.8389 (4)	0.9980 (3)	0.70238 (17)	0.0628 (8)
H28	0.7478	0.9972	0.6802	0.075*
C29	0.8153 (3)	0.7232 (2)	0.57102 (14)	0.0481 (6)
C30	0.9305 (4)	0.8340 (3)	0.54663 (16)	0.0670 (7)
H30	0.9631	0.9150	0.5731	0.080*
C31	0.9983 (4)	0.8262 (3)	0.48327 (16)	0.0773 (8)
H31	1.0765	0.9019	0.4679	0.093*
C32	0.9520 (4)	0.7095 (3)	0.44330 (17)	0.0757 (8)

H32	0.9956	0.7051	0.4000	0.091*
C33	0.8406 (5)	0.5990 (3)	0.46774 (18)	0.0904 (10)
H33	0.8091	0.5183	0.4410	0.108*
C34	0.7732 (4)	0.6044 (3)	0.53167 (16)	0.0789 (9)
H34	0.6992	0.5274	0.5480	0.095*
C35	0.5498 (3)	0.7466 (2)	0.63579 (14)	0.0464 (6)
C36	0.4941 (4)	0.7507 (3)	0.56753 (16)	0.0604 (7)
H36	0.5546	0.7508	0.5292	0.072*
C37	0.3480 (4)	0.7547 (3)	0.55584 (19)	0.0726 (9)
H37	0.3111	0.7566	0.5096	0.087*
C38	0.2587 (4)	0.7559 (3)	0.6109 (2)	0.0772 (10)
H38	0.1599	0.7564	0.6026	0.093*
C39	0.3152 (4)	0.7562 (4)	0.6786 (2)	0.0886 (11)
H39	0.2562	0.7606	0.7168	0.106*
C40	0.4580 (4)	0.7501 (4)	0.69101 (18)	0.0727 (9)
H40	0.4935	0.7483	0.7375	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0511 (2)	0.04317 (19)	0.0439 (2)	0.02402 (15)	0.00632 (14)	0.00292 (14)
S1	0.0506 (4)	0.0616 (4)	0.0663 (5)	0.0324 (4)	0.0010 (3)	−0.0061 (4)
P1	0.0432 (4)	0.0455 (4)	0.0410 (4)	0.0181 (3)	0.0044 (3)	0.0025 (3)
P2	0.0434 (4)	0.0419 (4)	0.0441 (4)	0.0224 (3)	0.0061 (3)	0.0038 (3)
N1	0.0483 (13)	0.0478 (13)	0.0477 (13)	0.0185 (11)	−0.0026 (10)	0.0012 (10)
N2	0.091 (2)	0.0479 (15)	0.085 (2)	0.0330 (15)	0.0004 (16)	−0.0061 (14)
C1	0.0646 (17)	0.0501 (16)	0.0392 (14)	0.0313 (14)	0.0034 (12)	0.0029 (12)
C2	0.0587 (19)	0.069 (2)	0.066 (2)	0.0175 (17)	−0.0041 (16)	−0.0010 (17)
C3	0.080 (3)	0.063 (2)	0.090 (3)	−0.001 (2)	−0.007 (2)	−0.008 (2)
C4	0.112 (3)	0.051 (2)	0.103 (3)	0.025 (2)	−0.001 (3)	−0.009 (2)
C5	0.0587 (17)	0.0444 (15)	0.0402 (14)	0.0170 (13)	−0.0016 (12)	0.0023 (11)
C6	0.090 (2)	0.064 (2)	0.064 (2)	0.0401 (18)	0.0112 (17)	0.0156 (16)
C7	0.142 (4)	0.073 (2)	0.088 (3)	0.063 (3)	0.002 (3)	0.013 (2)
C8	0.128 (4)	0.054 (2)	0.082 (3)	0.019 (2)	−0.010 (3)	0.0170 (19)
C9	0.083 (2)	0.058 (2)	0.073 (2)	0.0021 (19)	−0.0011 (19)	0.0115 (18)
C10	0.0599 (18)	0.0561 (18)	0.0577 (18)	0.0103 (15)	0.0012 (15)	0.0053 (14)
C11	0.0391 (14)	0.0517 (15)	0.0470 (15)	0.0164 (12)	0.0065 (11)	0.0075 (12)
C12	0.0494 (18)	0.075 (2)	0.071 (2)	0.0196 (16)	−0.0019 (15)	−0.0011 (17)
C13	0.0455 (19)	0.112 (3)	0.093 (3)	0.023 (2)	−0.0074 (18)	0.023 (2)
C14	0.056 (2)	0.109 (3)	0.111 (3)	0.050 (2)	0.023 (2)	0.036 (3)
C15	0.075 (2)	0.091 (3)	0.088 (3)	0.052 (2)	0.025 (2)	0.009 (2)
C16	0.0509 (17)	0.0708 (19)	0.0595 (18)	0.0298 (15)	0.0061 (14)	0.0011 (15)
C17	0.0368 (13)	0.0563 (16)	0.0443 (15)	0.0190 (12)	0.0064 (11)	0.0017 (12)
C18	0.0527 (17)	0.0684 (19)	0.0546 (18)	0.0200 (15)	0.0019 (14)	0.0086 (15)
C19	0.068 (2)	0.101 (3)	0.058 (2)	0.028 (2)	−0.0135 (17)	0.0042 (19)
C20	0.060 (2)	0.090 (3)	0.076 (2)	0.014 (2)	−0.0164 (18)	−0.016 (2)
C21	0.076 (2)	0.061 (2)	0.084 (3)	0.0115 (18)	−0.002 (2)	−0.0094 (19)
C22	0.0618 (19)	0.0542 (17)	0.0578 (18)	0.0147 (15)	−0.0005 (15)	0.0020 (14)

C23	0.0466 (15)	0.0428 (14)	0.0474 (15)	0.0184 (12)	0.0081 (12)	0.0050 (11)
C24	0.0468 (16)	0.0636 (19)	0.073 (2)	0.0239 (15)	0.0011 (15)	0.0033 (16)
C25	0.0542 (19)	0.084 (3)	0.086 (3)	0.0127 (18)	−0.0102 (17)	0.003 (2)
C26	0.084 (3)	0.060 (2)	0.083 (3)	0.000 (2)	−0.002 (2)	−0.0084 (19)
C27	0.103 (3)	0.0465 (18)	0.086 (3)	0.0284 (19)	0.002 (2)	−0.0038 (17)
C28	0.072 (2)	0.0522 (17)	0.068 (2)	0.0309 (16)	−0.0038 (16)	−0.0023 (15)
C29	0.0581 (14)	0.0497 (13)	0.0487 (14)	0.0332 (11)	0.0119 (11)	0.0103 (11)
C30	0.0793 (18)	0.0625 (15)	0.0639 (16)	0.0313 (14)	0.0215 (14)	0.0124 (13)
C31	0.090 (2)	0.0798 (17)	0.0699 (18)	0.0386 (16)	0.0323 (15)	0.0246 (14)
C32	0.104 (2)	0.0863 (18)	0.0624 (17)	0.0607 (16)	0.0352 (15)	0.0200 (14)
C33	0.140 (2)	0.0690 (17)	0.0681 (18)	0.0476 (17)	0.0362 (17)	0.0004 (15)
C34	0.118 (2)	0.0542 (15)	0.0610 (17)	0.0294 (15)	0.0303 (16)	0.0032 (13)
C35	0.0458 (14)	0.0447 (14)	0.0530 (15)	0.0222 (12)	0.0049 (12)	0.0072 (12)
C36	0.0608 (17)	0.0711 (19)	0.0539 (17)	0.0329 (15)	−0.0031 (14)	−0.0019 (15)
C37	0.0632 (19)	0.084 (2)	0.074 (2)	0.0354 (18)	−0.0173 (17)	0.0002 (18)
C38	0.0539 (18)	0.086 (2)	0.103 (3)	0.0386 (17)	0.0008 (18)	0.022 (2)
C39	0.074 (2)	0.131 (3)	0.095 (2)	0.071 (2)	0.0334 (19)	0.040 (2)
C40	0.071 (2)	0.113 (3)	0.0630 (19)	0.0626 (19)	0.0187 (16)	0.0266 (18)

Geometric parameters (Å, °)

Cu1—N1	2.139 (2)	C17—C18	1.385 (4)
Cu1—P2	2.2417 (7)	C18—C19	1.376 (4)
Cu1—P1	2.2557 (7)	C18—H18	0.9300
Cu1—S1	2.4023 (7)	C19—C20	1.368 (5)
S1—C1	1.715 (3)	C19—H19	0.9300
P1—C11	1.823 (3)	C20—C21	1.365 (5)
P1—C17	1.826 (3)	C20—H20	0.9300
P1—C5	1.836 (3)	C21—C22	1.384 (4)
P2—C23	1.820 (3)	C21—H21	0.9300
P2—C35	1.824 (3)	C22—H22	0.9300
P2—C29	1.825 (3)	C23—C28	1.383 (4)
N1—C2	1.329 (4)	C23—C24	1.389 (4)
N1—C1	1.357 (3)	C24—C25	1.379 (4)
N2—C4	1.315 (5)	C24—H24	0.9300
N2—C1	1.338 (3)	C25—C26	1.364 (5)
C2—C3	1.373 (5)	C25—H25	0.9300
C2—H2	0.9300	C26—C27	1.370 (5)
C3—C4	1.363 (5)	C26—H26	0.9300
C3—H3	0.9300	C27—C28	1.379 (4)
C4—H4	0.9300	C27—H27	0.9300
C5—C10	1.379 (4)	C28—H28	0.9300
C5—C6	1.380 (4)	C29—C34	1.373 (3)
C6—C7	1.393 (5)	C29—C30	1.378 (3)
C6—H6	0.9300	C30—C31	1.383 (3)
C7—C8	1.382 (6)	C30—H30	0.9300
C7—H7	0.9300	C31—C32	1.357 (3)
C8—C9	1.342 (6)	C31—H31	0.9300
C8—H8	0.9300	C32—C33	1.361 (4)

C9—C10	1.382 (4)	C32—H32	0.9300
C9—H9	0.9300	C33—C34	1.386 (3)
C10—H10	0.9300	C33—H33	0.9300
C11—C16	1.379 (4)	C34—H34	0.9300
C11—C12	1.386 (4)	C35—C40	1.377 (4)
C12—C13	1.384 (5)	C35—C36	1.380 (4)
C12—H12	0.9300	C36—C37	1.390 (4)
C13—C14	1.373 (5)	C36—H36	0.9300
C13—H13	0.9300	C37—C38	1.353 (5)
C14—C15	1.351 (5)	C37—H37	0.9300
C14—H14	0.9300	C38—C39	1.362 (5)
C15—C16	1.384 (4)	C38—H38	0.9300
C15—H15	0.9300	C39—C40	1.372 (4)
C16—H16	0.9300	C39—H39	0.9300
C17—C22	1.379 (4)	C40—H40	0.9300
N1—Cu1—P2	115.81 (6)	C22—C17—P1	117.5 (2)
N1—Cu1—P1	104.82 (6)	C18—C17—P1	124.2 (2)
P2—Cu1—P1	126.43 (3)	C19—C18—C17	120.6 (3)
N1—Cu1—S1	69.28 (6)	C19—C18—H18	119.7
P2—Cu1—S1	113.43 (3)	C17—C18—H18	119.7
P1—Cu1—S1	112.70 (3)	C20—C19—C18	120.8 (3)
C1—S1—Cu1	78.83 (9)	C20—C19—H19	119.6
C11—P1—C17	103.64 (12)	C18—C19—H19	119.6
C11—P1—C5	102.95 (13)	C21—C20—C19	119.2 (3)
C17—P1—C5	103.71 (12)	C21—C20—H20	120.4
C11—P1—Cu1	112.67 (9)	C19—C20—H20	120.4
C17—P1—Cu1	116.99 (8)	C20—C21—C22	120.8 (3)
C5—P1—Cu1	115.25 (9)	C20—C21—H21	119.6
C23—P2—C35	104.69 (12)	C22—C21—H21	119.6
C23—P2—C29	102.33 (12)	C17—C22—C21	120.4 (3)
C35—P2—C29	104.72 (12)	C17—C22—H22	119.8
C23—P2—Cu1	114.48 (9)	C21—C22—H22	119.8
C35—P2—Cu1	114.47 (9)	C28—C23—C24	118.2 (3)
C29—P2—Cu1	114.79 (8)	C28—C23—P2	124.7 (2)
C2—N1—C1	117.5 (3)	C24—C23—P2	117.1 (2)
C2—N1—Cu1	144.9 (2)	C25—C24—C23	120.7 (3)
C1—N1—Cu1	96.93 (16)	C25—C24—H24	119.7
C4—N2—C1	115.3 (3)	C23—C24—H24	119.7
N2—C1—N1	124.4 (3)	C26—C25—C24	120.1 (3)
N2—C1—S1	121.1 (2)	C26—C25—H25	119.9
N1—C1—S1	114.42 (19)	C24—C25—H25	120.0
N1—C2—C3	121.6 (3)	C25—C26—C27	120.2 (3)
N1—C2—H2	119.2	C25—C26—H26	119.9
C3—C2—H2	119.2	C27—C26—H26	119.9
C4—C3—C2	116.0 (3)	C26—C27—C28	120.0 (3)
C4—C3—H3	122.0	C26—C27—H27	120.0
C2—C3—H3	122.0	C28—C27—H27	120.0
N2—C4—C3	125.2 (3)	C27—C28—C23	120.8 (3)
N2—C4—H4	117.4	C27—C28—H28	119.6

C3—C4—H4	117.4	C23—C28—H28	119.6
C10—C5—C6	118.6 (3)	C34—C29—C30	118.1 (3)
C10—C5—P1	123.3 (2)	C34—C29—P2	118.7 (2)
C6—C5—P1	118.1 (2)	C30—C29—P2	122.9 (2)
C5—C6—C7	120.5 (3)	C29—C30—C31	120.8 (3)
C5—C6—H6	119.8	C29—C30—H30	119.6
C7—C6—H6	119.8	C31—C30—H30	119.6
C8—C7—C6	119.2 (4)	C32—C31—C30	120.8 (3)
C8—C7—H7	120.4	C32—C31—H31	119.6
C6—C7—H7	120.4	C30—C31—H31	119.6
C9—C8—C7	120.5 (4)	C31—C32—C33	118.7 (3)
C9—C8—H8	119.8	C31—C32—H32	120.6
C7—C8—H8	119.8	C33—C32—H32	120.6
C8—C9—C10	120.6 (4)	C32—C33—C34	121.3 (3)
C8—C9—H9	119.7	C32—C33—H33	119.4
C10—C9—H9	119.7	C34—C33—H33	119.4
C5—C10—C9	120.6 (3)	C29—C34—C33	120.2 (3)
C5—C10—H10	119.7	C29—C34—H34	119.9
C9—C10—H10	119.7	C33—C34—H34	119.9
C16—C11—C12	117.9 (3)	C40—C35—C36	117.9 (3)
C16—C11—P1	124.8 (2)	C40—C35—P2	117.9 (2)
C12—C11—P1	117.3 (2)	C36—C35—P2	124.0 (2)
C13—C12—C11	120.5 (3)	C35—C36—C37	120.2 (3)
C13—C12—H12	119.7	C35—C36—H36	119.9
C11—C12—H12	119.7	C37—C36—H36	119.9
C14—C13—C12	120.3 (3)	C38—C37—C36	120.8 (3)
C14—C13—H13	119.9	C38—C37—H37	119.6
C12—C13—H13	119.9	C36—C37—H37	119.6
C15—C14—C13	119.8 (3)	C37—C38—C39	119.2 (3)
C15—C14—H14	120.1	C37—C38—H38	120.4
C13—C14—H14	120.1	C39—C38—H38	120.4
C14—C15—C16	120.5 (3)	C38—C39—C40	120.7 (3)
C14—C15—H15	119.8	C38—C39—H39	119.7
C16—C15—H15	119.8	C40—C39—H39	119.7
C11—C16—C15	121.0 (3)	C39—C40—C35	121.1 (3)
C11—C16—H16	119.5	C39—C40—H40	119.4
C15—C16—H16	119.5	C35—C40—H40	119.4
C22—C17—C18	118.3 (3)		
N1—Cu1—S1—C1	−4.01 (11)	C11—C12—C13—C14	2.3 (5)
P2—Cu1—S1—C1	−114.09 (9)	C12—C13—C14—C15	−2.0 (6)
P1—Cu1—S1—C1	93.93 (9)	C13—C14—C15—C16	0.6 (6)
N1—Cu1—P1—C11	−89.40 (11)	C12—C11—C16—C15	−0.1 (4)
P2—Cu1—P1—C11	49.62 (10)	P1—C11—C16—C15	177.0 (2)
S1—Cu1—P1—C11	−162.77 (10)	C14—C15—C16—C11	0.4 (5)
N1—Cu1—P1—C17	150.64 (12)	C11—P1—C17—C22	−79.2 (2)
P2—Cu1—P1—C17	−70.34 (10)	C5—P1—C17—C22	173.5 (2)
S1—Cu1—P1—C17	77.26 (10)	Cu1—P1—C17—C22	45.4 (2)
N1—Cu1—P1—C5	28.35 (12)	C11—P1—C17—C18	101.6 (2)
P2—Cu1—P1—C5	167.37 (10)	C5—P1—C17—C18	−5.7 (3)

S1—Cu1—P1—C5	−45.03 (11)	Cu1—P1—C17—C18	−133.8 (2)
N1—Cu1—P2—C23	−172.61 (11)	C22—C17—C18—C19	−0.3 (4)
P1—Cu1—P2—C23	52.16 (10)	P1—C17—C18—C19	178.9 (2)
S1—Cu1—P2—C23	−95.24 (9)	C17—C18—C19—C20	0.3 (5)
N1—Cu1—P2—C35	66.51 (12)	C18—C19—C20—C21	0.2 (6)
P1—Cu1—P2—C35	−68.72 (10)	C19—C20—C21—C22	−0.7 (6)
S1—Cu1—P2—C35	143.87 (10)	C18—C17—C22—C21	−0.1 (4)
N1—Cu1—P2—C29	−54.66 (12)	P1—C17—C22—C21	−179.4 (2)
P1—Cu1—P2—C29	170.11 (10)	C20—C21—C22—C17	0.6 (5)
S1—Cu1—P2—C29	22.70 (10)	C35—P2—C23—C28	−11.3 (3)
P2—Cu1—N1—C2	−79.7 (4)	C29—P2—C23—C28	97.8 (3)
P1—Cu1—N1—C2	64.5 (4)	Cu1—P2—C23—C28	−137.4 (2)
S1—Cu1—N1—C2	173.5 (4)	C35—P2—C23—C24	169.1 (2)
P2—Cu1—N1—C1	111.82 (14)	C29—P2—C23—C24	−81.8 (2)
P1—Cu1—N1—C1	−104.06 (15)	Cu1—P2—C23—C24	43.0 (2)
S1—Cu1—N1—C1	5.01 (14)	C28—C23—C24—C25	−0.3 (4)
C4—N2—C1—N1	0.2 (5)	P2—C23—C24—C25	179.4 (2)
C4—N2—C1—S1	179.3 (3)	C23—C24—C25—C26	1.7 (5)
C2—N1—C1—N2	−0.7 (4)	C24—C25—C26—C27	−2.1 (6)
Cu1—N1—C1—N2	171.9 (2)	C25—C26—C27—C28	1.1 (6)
C2—N1—C1—S1	−179.8 (2)	C26—C27—C28—C23	0.3 (5)
Cu1—N1—C1—S1	−7.21 (19)	C24—C23—C28—C27	−0.7 (4)
Cu1—S1—C1—N2	−172.6 (2)	P2—C23—C28—C27	179.7 (2)
Cu1—S1—C1—N1	6.50 (17)	C23—P2—C29—C34	161.5 (3)
C1—N1—C2—C3	0.5 (5)	C35—P2—C29—C34	−89.5 (3)
Cu1—N1—C2—C3	−166.6 (3)	Cu1—P2—C29—C34	36.9 (3)
N1—C2—C3—C4	0.1 (6)	C23—P2—C29—C30	−12.7 (3)
C1—N2—C4—C3	0.5 (6)	C35—P2—C29—C30	96.4 (3)
C2—C3—C4—N2	−0.6 (6)	Cu1—P2—C29—C30	−137.3 (2)
C11—P1—C5—C10	−13.9 (3)	C34—C29—C30—C31	1.8 (5)
C17—P1—C5—C10	93.9 (2)	P2—C29—C30—C31	176.1 (3)
Cu1—P1—C5—C10	−136.9 (2)	C29—C30—C31—C32	0.5 (5)
C11—P1—C5—C6	164.6 (2)	C30—C31—C32—C33	−1.9 (6)
C17—P1—C5—C6	−87.7 (2)	C31—C32—C33—C34	0.8 (6)
Cu1—P1—C5—C6	41.5 (3)	C30—C29—C34—C33	−2.9 (5)
C10—C5—C6—C7	−0.4 (5)	P2—C29—C34—C33	−177.3 (3)
P1—C5—C6—C7	−179.0 (3)	C32—C33—C34—C29	1.6 (6)
C5—C6—C7—C8	0.8 (6)	C23—P2—C35—C40	−73.4 (3)
C6—C7—C8—C9	−1.3 (6)	C29—P2—C35—C40	179.3 (2)
C7—C8—C9—C10	1.4 (6)	Cu1—P2—C35—C40	52.8 (3)
C6—C5—C10—C9	0.5 (4)	C23—P2—C35—C36	111.3 (3)
P1—C5—C10—C9	178.9 (2)	C29—P2—C35—C36	4.0 (3)
C8—C9—C10—C5	−1.0 (5)	Cu1—P2—C35—C36	−122.5 (2)
C17—P1—C11—C16	1.8 (3)	C40—C35—C36—C37	−1.6 (5)
C5—P1—C11—C16	109.6 (3)	P2—C35—C36—C37	173.7 (2)
Cu1—P1—C11—C16	−125.6 (2)	C35—C36—C37—C38	0.6 (5)
C17—P1—C11—C12	178.9 (2)	C36—C37—C38—C39	1.5 (6)
C5—P1—C11—C12	−73.2 (2)	C37—C38—C39—C40	−2.6 (6)
Cu1—P1—C11—C12	51.5 (2)	C38—C39—C40—C35	1.5 (6)

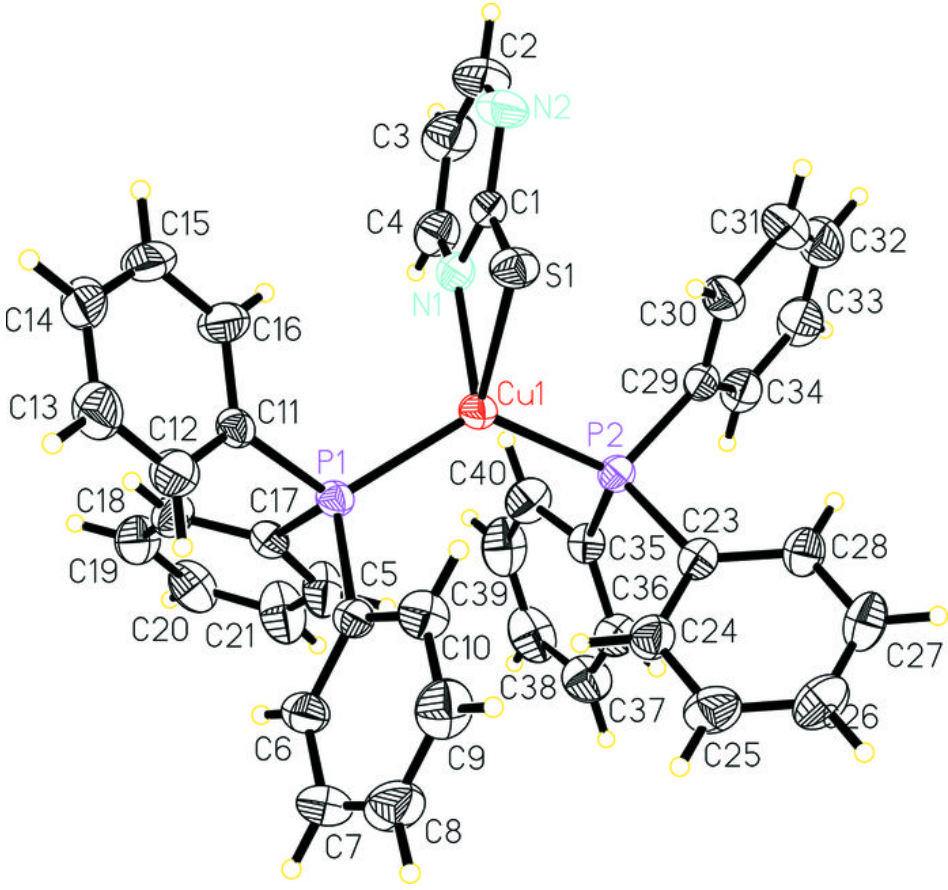
C16—C11—C12—C13	−1.2 (5)	C36—C35—C40—C39	0.6 (5)
P1—C11—C12—C13	−178.6 (3)	P2—C35—C40—C39	−175.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···S1	0.93	2.83	3.661 (3)	150
C13—H13···S1^{i}	0.93	2.73	3.613 (4)	159

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1


C2
N2
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C1
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C25
C7
C8

Fig. 2