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{(Hydrogen 2,2′,2″-boranetriyl)tris[6-*tert*-butyl-4-methylpyridazine-3(2*H*)-thione]-κ^3*H*,*S*,*S*′}-(triphenylphosphane-κ*P*)copper(I) chloroform disolvate

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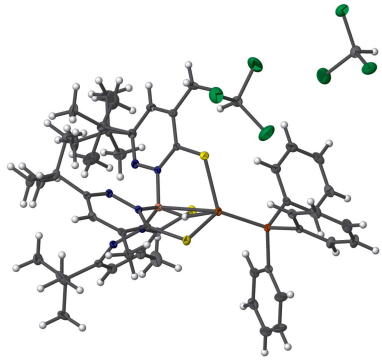
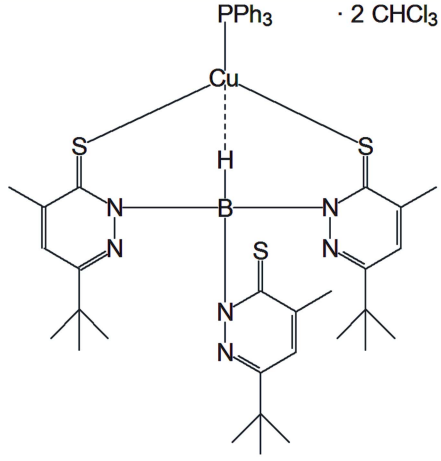
In the title complex, $[Cu(C_{27}H_{40}BN_6S_3)(C_{18}H_{15}P)]\cdot 2CHCl_3$, the Cu^I atom is surrounded in a trigonal-planar arrangement by the triphenylphosphane ligand and two of the three S atoms of the scorpionate ligand with an additional 3-center–2-electron B—H···Cu interaction, with the H atom as the apex of a pyramid [B—H = 1.140 (17) Å and Cu—H = 1.826 (16) Å].

3D view



Chemical scheme



Structure description

Soft scorpionate ligands have gained significant attention in synthetic inorganic chemistry over the last decades (Spicer & Reglinski, 2009; Reglinski & Spicer, 2015). For some years we have been investigating the behaviour of thiopyridazine-based hydroborates towards various metals and observed preferred metallaboratrane formation (Nuss *et al.*, 2011*a*,*b*; Holler *et al.*, 2016, 2017). However, the reaction of our soft scorpionate ligand potassium tris(6-*tert*-butyl-4-methylpyridazine-3(2*H*)-thione)borate (= $KTn^{Me,tBu}$) with copper(I) chloride in the presence of triphenylphosphane retained the borate ligand and led to the title compound. This represents an illustrative example where the scorpionate ligand binds in a κ^3-*H*,*S*,*S* fashion in contrast to our previously reported copper complexes with this ligand where we found exclusively boratranes (Cu—B bond). Copper complexes of the type presented here have previously been reported with similar ligands (Nuss *et al.*, 2011*a*, 2012; Owen *et al.*, 2013).

The asymmetric unit consists of one Cu^I complex, Fig. 1, and two chloroform solvate molecules. The scorpionate ligand is bonded to the Cu^I atom by two S atoms and by atom H1 bonded to B1 (Table 1); the triphenylphosphane ligand completes the coordination sphere. The Cu^I atom is situated 0.285 (3) Å above the trigonal plane defined by S1, S2,

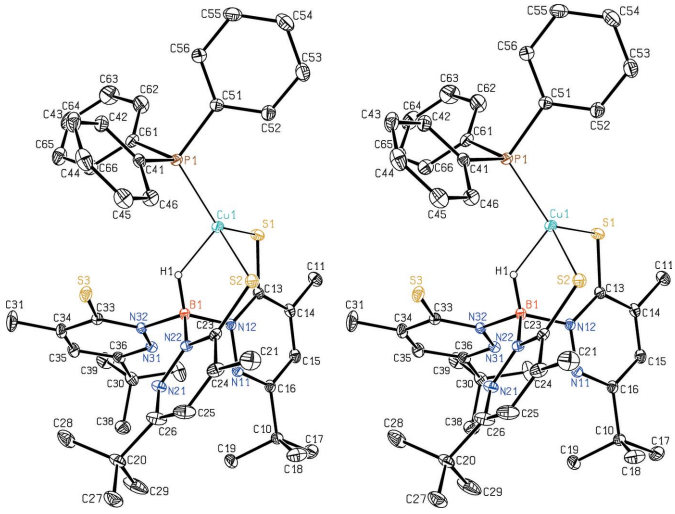


Figure 1
Stereoscopic plot of the molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level. Atom H1 is drawn with an arbitrary radius, the other H atoms as well as the less occupied orientation [39.3 (4)%] of the disordered *tert*-butyl group and the solvent molecules have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Cu1—H1	1.826 (16)	B1—N22	1.5598 (18)
Cu1—S1	2.2870 (4)	B1—N32	1.5612 (16)
Cu1—S2	2.3215 (4)	S1—C13	1.7112 (13)
Cu1—P1	2.2302 (4)	S2—C23	1.7187 (13)
B1—H1	1.140 (17)	S3—C33	1.6925 (13)
B1—N12	1.5737 (17)		
P1—Cu1—S1	125.136 (15)	C13—S1—Cu1	103.90 (5)
P1—Cu1—S2	121.306 (14)	N11—N12—C13	123.00 (11)
S1—Cu1—S2	108.874 (14)	N11—N12—B1	110.06 (10)
P1—Cu1—H1	112.5 (5)	C13—N12—B1	126.86 (11)
S1—Cu1—H1	88.0 (5)	C23—S2—Cu1	109.00 (4)
S2—Cu1—H1	88.7 (5)	N21—N22—C23	124.10 (11)
N12—B1—N22	106.44 (10)	N21—N22—B1	113.18 (10)
N12—B1—N32	110.37 (10)	C23—N22—B1	122.68 (11)
N22—B1—N32	109.22 (10)	N31—N32—C33	124.71 (10)
N12—B1—H1	115.3 (8)	N31—N32—B1	115.68 (10)
N22—B1—H1	111.4 (8)	C33—N32—B1	119.58 (10)
N32—B1—H1	104.0 (8)		

and P1, towards atom H1 as the apex of a pyramid (Table 1). The B1—H1—Cu1 angle is 132.6 (12)°, and the resulting overall coordination environment might be described as distorted tetrahedral.

The third S atom (S3) of the scorpionate ligand does not coordinate to the central atom [Cu1···S3 4.0976 (6) Å] and shows a distinctly shorter C—S distance than the others (Table 1). The triphenylphosphane ligand shows a staggered conformation [H1—Cu1—P1—C51 = −170.4 (6)°, S1—Cu1—P1—C41 = 176.17 (4)°, S2—Cu1—P1—C61 = −152.45 (5)°]. Non-classical hydrogen-bonding interactions (Table 2, Fig. 2) with C—H···S angles larger than 135° seem to consolidate the crystal packing and to play a role in the orientations of the solvent molecules as well as for the conformation of the copper(I) complex.

Synthesis and crystallization

A 25 ml Schlenk flask was charged with $KTn^{Me,tBu}$ (200.0 mg, 0.336 mmol), prepared by a reported procedure (Holler *et al.*, 2016), CuCl (33.0 mg, 0.336 mmol) and PPh_3 (176 mg,

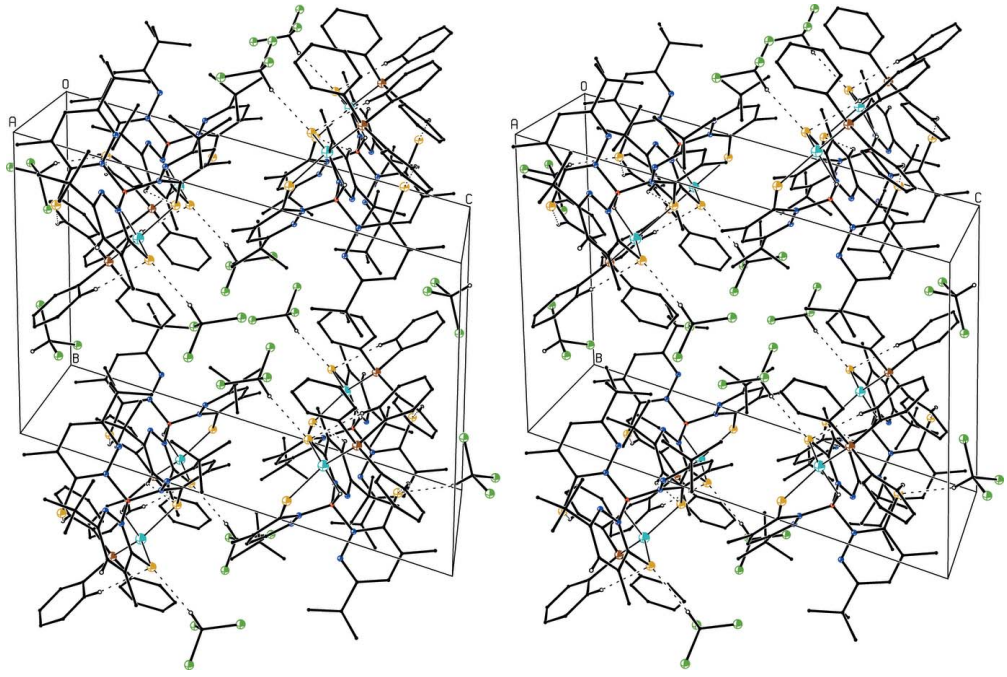


Figure 2
Stereoscopic plot of the packing of the title compound. The atoms are drawn with arbitrary radii. The non-classical C—H···S interactions (Table 2) were plotted with dashed lines. H atoms not involved as well as the less occupied orientations of the disordered *tert*-butyl groups were omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···S3^{i}	1.00	2.50	3.4366 (15)	156
C9—H9···S2	1.00	2.68	3.5468 (15)	145
C25—H25···S1^{ii}	0.95	2.70	3.4451 (15)	135
C46—H46···S2	0.95	2.82	3.7480 (15)	164
C66—H66···S3	0.95	2.85	3.7153 (16)	152

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

0.672 mmol). Anhydrous methanol (10 ml) was added *via* syringe whereupon the reaction turned into an orange suspension. The reaction mixture was stirred at room temperature for 3.5 h and then filtered over a pad of Celite, which was washed with methanol (2 × 10 ml). The yellow product was then eluted from the Celite with CH_2Cl_2 (30 ml). All volatiles were removed under reduced pressure to obtain the title compound as a yellow/orange powder (233 mg, 79%). Single crystals suitable for X-ray diffraction analysis were obtained *via* slow evaporation of a $CHCl_3$ solution. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60–7.51 (*m*, 6H), 7.36–7.31 (*m*, 9H), 7.04 (*q*, J = 0.9 Hz, 3H), 2.42 (*bs*, 9H), 1.02 (*s*, 27H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.8, 158.1, 147.2, 134.3, 129.6, 128.5, 121.0, 36.1, 29.2, 23.0.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The *tert*-butyl group bonded to C26 is disordered over two orientations [refined site occupation factors 0.607 (4) and 0.393 (4)]. No restraints were applied to the non-hydrogen atoms of this disordered group but in order to avoid a short intermolecular H···H contact of 1.99 Å, an anti-bumping restraint was applied between H371 and the disordered H atom H782′ having a site occupation factor of 0.393 (4) (*DFIX* in *SHELXL*; Sheldrick, 2015). Atom H1 bonded to B1 and coordinating to Cu1 was clearly identified in a difference Fourier map and was refined without any positional constraints with an individual isotropic displacement parameter.

Funding information

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_{27}H_{40}BN_6S_3)(C_{18}H_{15}P)]\cdot 2CHCl_3$
M_r	1120.18
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	9.6437 (5), 13.8713 (7), 20.7972 (10)
α, β, γ (°)	76.5300 (13), 81.7178 (14), 84.1877 (14)
V (Å^3)	2670.7 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.90
Crystal size (mm)	0.31 × 0.26 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.856, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	62765, 15577, 13590
R_{int}	0.033
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.085, 1.03
No. of reflections	15577
No. of parameters	663
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.25, −0.76

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and modified *ORTEP* (Johnson, 1965).

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full crystallographic data

IUCrData (2017). **2**, x171772 [https://doi.org/10.1107/S2414314617017722]

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Crystal data

$[Cu(C_{27}H_{40}BN_6S_3)(C_{18}H_{15}P)]\cdot 2CHCl_3$
M_r = 1120.18
Triclinic, $P\overline{1}$
a = 9.6437 (5) Å
b = 13.8713 (7) Å
c = 20.7972 (10) Å
α = 76.5300 (13)°
β = 81.7178 (14)°
γ = 84.1877 (14)°
V = 2670.7 (2) Å^3
Z = 2
$F(000)$ = 1160
D_x = 1.393 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9712 reflections
θ = 2.8–30.7°
μ = 0.90 mm^{-1}
T = 100 K
Plate, orange
0.31 × 0.26 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: Incoatec microfocus sealed tube
Multilayer monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.856, T_{max} = 1.000
62765 measured reflections
15577 independent reflections
13590 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 30.0°, θ_{min} = 2.5°
h = −13→13
k = −19→19
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.03
15577 reflections
663 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 1.5295P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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.
The non-hydrogen atoms were refined with anisotropic displacement parameters without any constraints.
The tert-butyl group bonded to C26 was disordered over two orientations and refined with site occupation factors of 0.607 (4) and 0.393 (4), respectively. No restraints were applied to the non-hydrogen atoms of this disordered group but in order to avoid a short intermolecular H···H contact of 1.99 Å an anti-bumping restraint was applied between H371 and the disordered H atom H782′ having a site occupation factor of 0.393 (4) (DFIX of SHELXL).
The H atom H1 bonded to B1 and co-ordinated to Cu1 was clearly identified in a difference Fourier map and was refined without any positional constraints with an individual isotropic displacement parameter.
The H atoms of the pyridazine rings were put at the external bisectors of the C-C-C angles at C-H distances of 0.95 Å and individual isotropic displacement parameters were refined for these H atoms (AFIX 43 of SHELXL).
The H atoms of the phenyl rings were put at the external bisectors of the C-C-C angles at C-H distances of 0.95 Å and common isotropic displacement parameters were refined for the H atoms of the same phenyl group (AFIX 43 of SHELXL).
The H atoms of the methyl groups were refined with common isotropic displacement parameters for the H atoms of the same group and idealized geometries with tetrahedral angles, enabling rotation around the C-C bond, and C-H distances of 0.98 Å (AFIX 137 of SHELXL).
The H atoms of the solvent molecules were refined with individual isotropic displacement parameters and all Cl-C-H angles equal at a C-H distance of 1.00 Å (AFIX 13 of SHELXL).
The largest peaks in a final difference Fourier map (0.69 - 1.25 $e\text{Å}^{-3}$) were in the vicinity (0.63 - 0.76 Å) of the Cl atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.97985 (2)	0.78129 (2)	0.70928 (2)	0.01169 (4)	
B1	0.81901 (15)	0.95096 (10)	0.72202 (7)	0.0102 (2)	
H1	0.8899 (18)	0.8839 (12)	0.7436 (8)	0.011 (4)*	
S1	1.11555 (3)	0.89463 (2)	0.63607 (2)	0.01430 (6)	
N11	0.77029 (12)	1.07717 (8)	0.62536 (5)	0.0114 (2)	
N12	0.87133 (12)	1.00774 (8)	0.64913 (5)	0.01013 (19)	
C13	1.00037 (13)	0.99535 (9)	0.61417 (6)	0.0110 (2)	
C14	1.03792 (14)	1.07065 (9)	0.55534 (6)	0.0127 (2)	
C15	0.93655 (15)	1.14157 (9)	0.53303 (6)	0.0139 (2)	
H15	0.9581	1.1917	0.4940	0.018 (4)*	
C16	0.79898 (14)	1.14034 (9)	0.56812 (6)	0.0120 (2)	
C10	0.67398 (14)	1.20933 (9)	0.54374 (6)	0.0136 (2)	
C17	0.71936 (17)	1.28707 (11)	0.48061 (7)	0.0223 (3)	
H171	0.7887	1.3273	0.4900	0.027 (3)*	
H172	0.6373	1.3301	0.4664	0.027 (3)*	
H173	0.7611	1.2535	0.4451	0.027 (3)*	
C18	0.56603 (17)	1.14583 (11)	0.52864 (9)	0.0239 (3)	
H181	0.6078	1.1137	0.4925	0.029 (3)*	
H182	0.4830	1.1884	0.5152	0.029 (3)*	
H183	0.5386	1.0950	0.5686	0.029 (3)*	

C19	0.60608 (18)	1.26300 (11)	0.59843 (7)	0.0231 (3)	
H191	0.5808	1.2139	0.6397	0.033 (3)*	
H192	0.5214	1.3028	0.5843	0.033 (3)*	
H193	0.6727	1.3066	0.6063	0.033 (3)*	
C11	1.18409 (15)	1.06885 (10)	0.51914 (7)	0.0175 (3)	
H111	1.1916	1.1257	0.4810	0.028 (3)*	
H112	1.2048	1.0070	0.5034	0.028 (3)*	
H113	1.2514	1.0727	0.5494	0.028 (3)*	
S2	0.77795 (4)	0.77010 (2)	0.66343 (2)	0.01401 (6)	
N21	0.56577 (12)	0.98183 (8)	0.74507 (6)	0.0138 (2)	
N22	0.66805 (11)	0.92110 (8)	0.72053 (5)	0.01051 (19)	
C23	0.64366 (14)	0.84389 (9)	0.69495 (6)	0.0115 (2)	
C24	0.50042 (15)	0.82529 (10)	0.69524 (7)	0.0165 (3)	
C25	0.39772 (15)	0.88455 (11)	0.72248 (8)	0.0215 (3)	
H25	0.3018	0.8721	0.7249	0.028 (5)*	
C26	0.43399 (15)	0.96432 (10)	0.74700 (8)	0.0197 (3)	
C20	0.3273 (4)	1.0320 (3)	0.78506 (19)	0.0169 (7)	0.607 (4)
C27	0.1756 (9)	1.0055 (7)	0.7880 (4)	0.0254 (13)	0.607 (4)
H271	0.1116	1.0496	0.8111	0.026 (5)*	0.607 (4)
H272	0.1659	0.9364	0.8122	0.026 (5)*	0.607 (4)
H273	0.1523	1.0135	0.7426	0.026 (5)*	0.607 (4)
C28	0.3611 (3)	1.0235 (2)	0.85632 (14)	0.0260 (6)	0.607 (4)
H281	0.2954	1.0685	0.8779	0.038 (6)*	0.607 (4)
H282	0.4574	1.0416	0.8546	0.038 (6)*	0.607 (4)
H283	0.3520	0.9550	0.8818	0.038 (6)*	0.607 (4)
C29	0.3454 (3)	1.1392 (2)	0.74572 (18)	0.0365 (9)	0.607 (4)
H291	0.3285	1.1450	0.6996	0.034 (6)*	0.607 (4)
H292	0.4411	1.1565	0.7463	0.034 (6)*	0.607 (4)
H293	0.2780	1.1845	0.7662	0.034 (6)*	0.607 (4)
C70	0.3255 (7)	1.0446 (5)	0.7600 (3)	0.0190 (11)	0.393 (4)
C77	0.3864 (5)	1.1067 (4)	0.7986 (3)	0.0405 (15)	0.393 (4)
H771	0.4152	1.0639	0.8398	0.054 (7)*	0.393 (4)
H772	0.3152	1.1579	0.8096	0.054 (7)*	0.393 (4)
H773	0.4681	1.1383	0.7714	0.054 (7)*	0.393 (4)
C78	0.2744 (5)	1.1114 (3)	0.6968 (2)	0.0288 (10)	0.393 (4)
H781	0.3522	1.1189	0.6605	0.054 (7)*	0.393 (4)
H782	0.2405	1.1769	0.7054	0.054 (7)*	0.393 (4)
H783	0.1978	1.0811	0.6842	0.054 (7)*	0.393 (4)
C79	0.1989 (15)	0.9928 (12)	0.8021 (7)	0.032 (2)	0.393 (4)
H791	0.1578	0.9556	0.7758	0.054 (7)*	0.393 (4)
H792	0.1285	1.0427	0.8157	0.054 (7)*	0.393 (4)
H793	0.2295	0.9470	0.8419	0.054 (7)*	0.393 (4)
C21	0.46520 (17)	0.74187 (11)	0.66688 (8)	0.0235 (3)	
H211	0.3634	0.7364	0.6745	0.029 (3)*	
H212	0.5124	0.6794	0.6888	0.029 (3)*	
H213	0.4969	0.7554	0.6189	0.029 (3)*	
S3	0.73473 (4)	0.86461 (2)	0.86796 (2)	0.01707 (7)	
N31	0.84628 (11)	1.11562 (8)	0.74394 (5)	0.01107 (19)	

N32	0.81238 (11)	1.02062 (8)	0.77167 (5)	0.01004 (19)
C33	0.77875 (14)	0.98333 (9)	0.83847 (6)	0.0130 (2)
C34	0.78018 (16)	1.05114 (10)	0.88167 (7)	0.0172 (3)
C35	0.81160 (16)	1.14649 (10)	0.85337 (7)	0.0177 (3)
H35	0.8110	1.1927	0.8807	0.026 (5)*
C36	0.84533 (14)	1.17743 (9)	0.78318 (7)	0.0128 (2)
C30	0.87687 (15)	1.28457 (10)	0.74976 (7)	0.0161 (3)
C37	0.94920 (19)	1.29169 (11)	0.67840 (8)	0.0271 (3)
H371	1.0370	1.2494	0.6791	0.035 (3)*
H372	0.9697	1.3608	0.6582	0.035 (3)*
H373	0.8871	1.2694	0.6522	0.035 (3)*
C38	0.73617 (17)	1.34774 (11)	0.74902 (8)	0.0223 (3)
H381	0.6740	1.3220	0.7246	0.031 (3)*
H382	0.7530	1.4169	0.7272	0.031 (3)*
H383	0.6919	1.3445	0.7949	0.031 (3)*
C39	0.97291 (17)	1.32434 (12)	0.78925 (9)	0.0249 (3)
H391	0.9246	1.3251	0.8340	0.034 (3)*
H392	0.9954	1.3920	0.7661	0.034 (3)*
H393	1.0598	1.2813	0.7928	0.034 (3)*
C31	0.7468 (2)	1.01526 (12)	0.95572 (7)	0.0291 (4)
H311	0.7536	1.0696	0.9777	0.037 (3)*
H312	0.8137	0.9598	0.9716	0.037 (3)*
H313	0.6512	0.9930	0.9661	0.037 (3)*
P1	1.05935 (4)	0.65750 (2)	0.78750 (2)	0.01079 (6)
C41	0.92798 (14)	0.58098 (9)	0.84384 (6)	0.0128 (2)
C42	0.96040 (16)	0.51642 (10)	0.90314 (7)	0.0164 (3)
H42	1.0504	0.5153	0.9169	0.025 (2)*
C43	0.86124 (17)	0.45372 (11)	0.94204 (7)	0.0205 (3)
H43	0.8840	0.4098	0.9821	0.025 (2)*
C44	0.72889 (17)	0.45530 (11)	0.92231 (8)	0.0219 (3)
H44	0.6616	0.4123	0.9488	0.025 (2)*
C45	0.69544 (16)	0.51969 (11)	0.86409 (8)	0.0217 (3)
H45	0.6049	0.5210	0.8508	0.025 (2)*
C46	0.79459 (15)	0.58280 (10)	0.82479 (7)	0.0174 (3)
H46	0.7710	0.6270	0.7850	0.025 (2)*
C51	1.17433 (14)	0.56437 (9)	0.75231 (6)	0.0125 (2)
C52	1.17805 (15)	0.56859 (10)	0.68438 (7)	0.0159 (2)
H52	1.1259	0.6209	0.6579	0.025 (2)*
C53	1.25761 (17)	0.49678 (11)	0.65509 (7)	0.0214 (3)
H53	1.2587	0.4999	0.6089	0.025 (2)*
C54	1.33506 (17)	0.42092 (11)	0.69336 (8)	0.0239 (3)
H54	1.3895	0.3721	0.6734	0.025 (2)*
C55	1.33289 (17)	0.41637 (11)	0.76104 (8)	0.0228 (3)
H55	1.3867	0.3647	0.7872	0.025 (2)*
C56	1.25244 (16)	0.48698 (10)	0.79049 (7)	0.0185 (3)
H56	1.2503	0.4828	0.8369	0.025 (2)*
C61	1.16102 (15)	0.69298 (9)	0.84535 (6)	0.0138 (2)
C62	1.30710 (17)	0.68154 (12)	0.83999 (8)	0.0234 (3)

H62	1.3580	0.6504	0.8068	0.030 (2)*
C63	1.37949 (18)	0.71547 (14)	0.88305 (9)	0.0301 (4)
H63	1.4792	0.7075	0.8790	0.030 (2)*
C64	1.30584 (19)	0.76081 (12)	0.93169 (8)	0.0258 (3)
H64	1.3550	0.7833	0.9612	0.030 (2)*
C65	1.16061 (18)	0.77337 (11)	0.93718 (7)	0.0226 (3)
H65	1.1103	0.8049	0.9703	0.030 (2)*
C66	1.08801 (16)	0.73982 (10)	0.89422 (7)	0.0184 (3)
H66	0.9884	0.7488	0.8981	0.030 (2)*
C8	0.32427 (17)	0.25592 (11)	0.96738 (7)	0.0205 (3)
H8	0.3160	0.2030	1.0093	0.024 (5)*
Cl81	0.32920 (6)	0.37050 (4)	0.98866 (3)	0.04140 (12)
Cl82	0.17658 (4)	0.25670 (3)	0.92608 (2)	0.02814 (8)
Cl83	0.48058 (4)	0.22845 (3)	0.91718 (2)	0.02899 (9)
C9	0.76705 (16)	0.62214 (11)	0.54650 (8)	0.0214 (3)
H9	0.7337	0.6777	0.5693	0.027 (5)*
Cl91	0.63549 (6)	0.53827 (4)	0.56429 (3)	0.05072 (14)
Cl92	0.92293 (6)	0.56614 (5)	0.57672 (3)	0.05035 (14)
Cl93	0.79802 (6)	0.67288 (3)	0.46038 (2)	0.03587 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01435 (8)	0.00921 (7)	0.01153 (8)	0.00116 (5)	−0.00280 (6)	−0.00243 (5)
B1	0.0118 (6)	0.0096 (5)	0.0096 (6)	−0.0017 (5)	−0.0006 (5)	−0.0027 (4)
S1	0.01217 (15)	0.01301 (14)	0.01599 (15)	0.00139 (11)	0.00052 (11)	−0.00207 (11)
N11	0.0134 (5)	0.0097 (4)	0.0113 (5)	0.0004 (4)	−0.0019 (4)	−0.0032 (4)
N12	0.0123 (5)	0.0086 (4)	0.0097 (5)	−0.0006 (4)	−0.0010 (4)	−0.0029 (4)
C13	0.0121 (6)	0.0100 (5)	0.0115 (5)	−0.0014 (4)	−0.0007 (4)	−0.0040 (4)
C14	0.0145 (6)	0.0121 (5)	0.0118 (5)	−0.0033 (4)	0.0015 (4)	−0.0045 (4)
C15	0.0186 (6)	0.0115 (5)	0.0109 (5)	−0.0029 (5)	0.0011 (5)	−0.0019 (4)
C16	0.0158 (6)	0.0098 (5)	0.0111 (5)	−0.0008 (4)	−0.0015 (4)	−0.0039 (4)
C10	0.0164 (6)	0.0109 (5)	0.0123 (6)	0.0017 (4)	−0.0016 (5)	−0.0016 (4)
C17	0.0249 (8)	0.0200 (7)	0.0169 (6)	0.0029 (6)	−0.0019 (6)	0.0043 (5)
C18	0.0198 (7)	0.0190 (7)	0.0344 (8)	0.0016 (5)	−0.0110 (6)	−0.0054 (6)
C19	0.0299 (8)	0.0212 (7)	0.0165 (6)	0.0110 (6)	−0.0021 (6)	−0.0064 (5)
C11	0.0159 (7)	0.0166 (6)	0.0182 (6)	−0.0031 (5)	0.0045 (5)	−0.0034 (5)
S2	0.01590 (15)	0.01419 (14)	0.01428 (14)	0.00043 (11)	−0.00433 (11)	−0.00699 (11)
N21	0.0118 (5)	0.0113 (5)	0.0178 (5)	0.0012 (4)	−0.0009 (4)	−0.0035 (4)
N22	0.0111 (5)	0.0088 (4)	0.0112 (5)	−0.0001 (4)	−0.0019 (4)	−0.0013 (4)
C23	0.0141 (6)	0.0101 (5)	0.0102 (5)	−0.0013 (4)	−0.0040 (4)	−0.0004 (4)
C24	0.0159 (6)	0.0139 (6)	0.0211 (6)	−0.0024 (5)	−0.0073 (5)	−0.0030 (5)
C25	0.0121 (6)	0.0176 (6)	0.0365 (8)	−0.0015 (5)	−0.0078 (6)	−0.0062 (6)
C26	0.0124 (6)	0.0141 (6)	0.0327 (8)	0.0007 (5)	−0.0027 (5)	−0.0063 (5)
C20	0.0139 (13)	0.0119 (13)	0.0218 (18)	0.0020 (9)	0.0036 (16)	−0.0024 (15)
C27	0.011 (2)	0.037 (4)	0.031 (3)	0.001 (2)	−0.0012 (17)	−0.016 (3)
C28	0.0229 (13)	0.0295 (13)	0.0315 (14)	0.0026 (10)	−0.0015 (10)	−0.0217 (11)
C29	0.0288 (16)	0.0171 (12)	0.051 (2)	0.0092 (11)	0.0146 (14)	0.0017 (12)

C70	0.0122 (19)	0.023 (3)	0.021 (3)	0.0010 (16)	0.000 (2)	−0.006 (3)
C77	0.026 (2)	0.055 (3)	0.052 (3)	0.017 (2)	−0.011 (2)	−0.041 (3)
C78	0.027 (2)	0.0207 (19)	0.034 (2)	0.0101 (16)	−0.0042 (17)	−0.0019 (16)
C79	0.021 (6)	0.029 (3)	0.038 (6)	0.006 (3)	0.008 (3)	−0.001 (4)
C21	0.0211 (7)	0.0217 (7)	0.0328 (8)	−0.0054 (6)	−0.0091 (6)	−0.0115 (6)
S3	0.02550 (18)	0.01294 (14)	0.01112 (14)	−0.00156 (12)	−0.00065 (12)	−0.00027 (11)
N31	0.0105 (5)	0.0101 (4)	0.0129 (5)	−0.0012 (4)	−0.0010 (4)	−0.0034 (4)
N32	0.0110 (5)	0.0096 (4)	0.0102 (5)	−0.0006 (4)	−0.0015 (4)	−0.0035 (4)
C33	0.0145 (6)	0.0129 (5)	0.0113 (5)	0.0011 (4)	−0.0018 (4)	−0.0029 (4)
C34	0.0227 (7)	0.0185 (6)	0.0115 (6)	0.0011 (5)	−0.0019 (5)	−0.0065 (5)
C35	0.0228 (7)	0.0176 (6)	0.0156 (6)	0.0003 (5)	−0.0031 (5)	−0.0097 (5)
C36	0.0110 (6)	0.0128 (5)	0.0164 (6)	−0.0001 (4)	−0.0018 (5)	−0.0068 (5)
C30	0.0179 (7)	0.0122 (5)	0.0197 (6)	−0.0032 (5)	0.0002 (5)	−0.0072 (5)
C37	0.0391 (10)	0.0173 (7)	0.0240 (7)	−0.0121 (6)	0.0116 (7)	−0.0081 (6)
C38	0.0258 (8)	0.0163 (6)	0.0257 (7)	0.0033 (5)	−0.0052 (6)	−0.0074 (5)
C39	0.0233 (8)	0.0214 (7)	0.0352 (8)	−0.0065 (6)	−0.0047 (6)	−0.0143 (6)
C31	0.0527 (11)	0.0241 (7)	0.0110 (6)	−0.0010 (7)	−0.0016 (7)	−0.0068 (5)
P1	0.01194 (15)	0.00974 (13)	0.01067 (14)	−0.00042 (11)	−0.00267 (11)	−0.00161 (11)
C41	0.0150 (6)	0.0111 (5)	0.0126 (5)	−0.0013 (4)	0.0004 (5)	−0.0041 (4)
C42	0.0207 (7)	0.0145 (6)	0.0140 (6)	−0.0023 (5)	−0.0020 (5)	−0.0031 (5)
C43	0.0313 (8)	0.0154 (6)	0.0136 (6)	−0.0050 (6)	0.0011 (5)	−0.0018 (5)
C44	0.0260 (8)	0.0180 (6)	0.0216 (7)	−0.0093 (6)	0.0072 (6)	−0.0068 (5)
C45	0.0172 (7)	0.0232 (7)	0.0260 (7)	−0.0059 (5)	0.0005 (6)	−0.0082 (6)
C46	0.0167 (7)	0.0173 (6)	0.0181 (6)	−0.0022 (5)	−0.0023 (5)	−0.0031 (5)
C51	0.0121 (6)	0.0107 (5)	0.0144 (6)	−0.0014 (4)	−0.0012 (4)	−0.0023 (4)
C52	0.0193 (7)	0.0139 (6)	0.0145 (6)	−0.0021 (5)	−0.0021 (5)	−0.0027 (5)
C53	0.0294 (8)	0.0186 (6)	0.0159 (6)	−0.0016 (6)	0.0016 (6)	−0.0059 (5)
C54	0.0249 (8)	0.0190 (7)	0.0254 (7)	0.0015 (6)	0.0070 (6)	−0.0075 (6)
C55	0.0208 (7)	0.0188 (6)	0.0245 (7)	0.0066 (5)	0.0000 (6)	−0.0014 (5)
C56	0.0195 (7)	0.0181 (6)	0.0158 (6)	0.0034 (5)	−0.0016 (5)	−0.0022 (5)
C61	0.0172 (6)	0.0117 (5)	0.0130 (6)	−0.0021 (5)	−0.0051 (5)	−0.0015 (4)
C62	0.0189 (7)	0.0309 (8)	0.0243 (7)	−0.0022 (6)	−0.0052 (6)	−0.0122 (6)
C63	0.0211 (8)	0.0381 (9)	0.0371 (9)	−0.0035 (7)	−0.0126 (7)	−0.0141 (7)
C64	0.0355 (9)	0.0232 (7)	0.0233 (7)	−0.0069 (6)	−0.0153 (7)	−0.0052 (6)
C65	0.0349 (9)	0.0169 (6)	0.0182 (7)	−0.0044 (6)	−0.0061 (6)	−0.0059 (5)
C66	0.0218 (7)	0.0151 (6)	0.0197 (6)	−0.0018 (5)	−0.0051 (5)	−0.0050 (5)
C8	0.0254 (8)	0.0225 (7)	0.0133 (6)	0.0024 (6)	−0.0013 (5)	−0.0056 (5)
Cl81	0.0545 (3)	0.0314 (2)	0.0459 (3)	0.0054 (2)	−0.0107 (2)	−0.0249 (2)
Cl82	0.02276 (19)	0.0348 (2)	0.02579 (18)	0.00148 (15)	−0.00454 (14)	−0.00522 (15)
Cl83	0.02298 (19)	0.0426 (2)	0.02461 (18)	0.00282 (16)	−0.00221 (14)	−0.01652 (16)
C9	0.0211 (7)	0.0201 (7)	0.0245 (7)	−0.0008 (5)	−0.0039 (6)	−0.0078 (6)
Cl91	0.0370 (3)	0.0318 (2)	0.0801 (4)	−0.0163 (2)	−0.0030 (3)	−0.0025 (2)
Cl92	0.0345 (3)	0.0562 (3)	0.0576 (3)	0.0084 (2)	−0.0212 (2)	−0.0026 (3)
Cl93	0.0485 (3)	0.0355 (2)	0.02295 (19)	−0.00079 (19)	−0.00171 (18)	−0.00773 (16)

Geometric parameters (Å, º)

Cu1—H1	1.826 (16)	C21—H213	0.98
Cu1—S1	2.2870 (4)	S3—C33	1.6925 (13)
Cu1—S2	2.3215 (4)	N31—C36	1.3128 (15)
Cu1—P1	2.2302 (4)	N31—N32	1.3619 (14)
B1—H1	1.140 (17)	N32—C33	1.3682 (16)
B1—N12	1.5737 (17)	C33—C34	1.4465 (17)
B1—N22	1.5598 (18)	C34—C35	1.362 (2)
B1—N32	1.5612 (16)	C34—C31	1.502 (2)
S1—C13	1.7112 (13)	C35—C36	1.4216 (19)
N11—C16	1.3152 (16)	C35—H35	0.95
N11—N12	1.3595 (15)	C36—C30	1.5276 (18)
N12—C13	1.3642 (16)	C30—C37	1.532 (2)
C13—C14	1.4397 (17)	C30—C38	1.539 (2)
C14—C15	1.3645 (19)	C30—C39	1.540 (2)
C14—C11	1.5001 (19)	C37—H371	0.98
C15—C16	1.4188 (19)	C37—H372	0.98
C15—H15	0.95	C37—H373	0.98
C16—C10	1.5305 (18)	C38—H381	0.98
C10—C17	1.5326 (19)	C38—H382	0.98
C10—C19	1.5355 (19)	C38—H383	0.98
C10—C18	1.538 (2)	C39—H391	0.98
C17—H171	0.98	C39—H392	0.98
C17—H172	0.98	C39—H393	0.98
C17—H173	0.98	C31—H311	0.98
C18—H181	0.98	C31—H312	0.98
C18—H182	0.98	C31—H313	0.98
C18—H183	0.98	P1—C51	1.8304 (13)
C19—H191	0.98	P1—C61	1.8341 (13)
C19—H192	0.98	P1—C41	1.8357 (14)
C19—H193	0.98	C41—C46	1.3956 (19)
C11—H111	0.98	C41—C42	1.4003 (18)
C11—H112	0.98	C42—C43	1.394 (2)
C11—H113	0.98	C42—H42	0.95
S2—C23	1.7187 (13)	C43—C44	1.392 (2)
N21—C26	1.3111 (18)	C43—H43	0.95
N21—N22	1.3528 (15)	C44—C45	1.385 (2)
N22—C23	1.3557 (15)	C44—H44	0.95
C23—C24	1.4296 (19)	C45—C46	1.400 (2)
C24—C25	1.367 (2)	C45—H45	0.95
C24—C21	1.5025 (19)	C46—H46	0.95
C25—C26	1.414 (2)	C51—C52	1.3957 (18)
C25—H25	0.95	C51—C56	1.4006 (19)
C26—C70	1.494 (7)	C52—C53	1.3948 (19)
C26—C20	1.575 (4)	C52—H52	0.95
C20—C27	1.534 (10)	C53—C54	1.386 (2)
C20—C29	1.535 (5)	C53—H53	0.95

C20—C28	1.538 (5)	C54—C55	1.391 (2)
C27—H271	0.98	C54—H54	0.95
C27—H272	0.98	C55—C56	1.387 (2)
C27—H273	0.98	C55—H55	0.95
C28—H281	0.98	C56—H56	0.95
C28—H282	0.98	C61—C62	1.393 (2)
C28—H283	0.98	C61—C66	1.3999 (19)
C29—H291	0.98	C62—C63	1.398 (2)
C29—H292	0.98	C62—H62	0.95
C29—H293	0.98	C63—C64	1.387 (2)
C70—C77	1.513 (8)	C63—H63	0.95
C70—C79	1.533 (17)	C64—C65	1.385 (2)
C70—C78	1.535 (7)	C64—H64	0.95
C77—H771	0.98	C65—C66	1.395 (2)
C77—H772	0.98	C65—H65	0.95
C77—H773	0.98	C66—H66	0.95
C78—H781	0.98	C8—Cl81	1.7532 (15)
C78—H782	0.98	C8—Cl82	1.7638 (16)
C78—H783	0.98	C8—Cl83	1.7672 (16)
C79—H791	0.98	C8—H8	1.00
C79—H792	0.98	C9—Cl91	1.7502 (16)
C79—H793	0.98	C9—Cl92	1.7512 (16)
C21—H211	0.98	C9—Cl93	1.7589 (16)
C21—H212	0.98	C9—H9	1.00

P1—Cu1—S1	125.136 (15)	H792—C79—H793	109.5
P1—Cu1—S2	121.306 (14)	C24—C21—H211	109.5
S1—Cu1—S2	108.874 (14)	C24—C21—H212	109.5
P1—Cu1—H1	112.5 (5)	H211—C21—H212	109.5
S1—Cu1—H1	88.0 (5)	C24—C21—H213	109.5
S2—Cu1—H1	88.7 (5)	H211—C21—H213	109.5
N12—B1—N22	106.44 (10)	H212—C21—H213	109.5
N12—B1—N32	110.37 (10)	C36—N31—N32	118.68 (11)
N22—B1—N32	109.22 (10)	N31—N32—C33	124.71 (10)
N12—B1—H1	115.3 (8)	N31—N32—B1	115.68 (10)
N22—B1—H1	111.4 (8)	C33—N32—B1	119.58 (10)
N32—B1—H1	104.0 (8)	N32—C33—C34	116.48 (11)
C13—S1—Cu1	103.90 (5)	N32—C33—S3	121.14 (9)
C16—N11—N12	119.59 (11)	C34—C33—S3	122.37 (10)
N11—N12—C13	123.00 (11)	C35—C34—C33	118.37 (12)
N11—N12—B1	110.06 (10)	C35—C34—C31	121.99 (12)
C13—N12—B1	126.86 (11)	C33—C34—C31	119.64 (13)
N12—C13—C14	117.30 (11)	C34—C35—C36	120.49 (12)
N12—C13—S1	123.24 (9)	C34—C35—H35	119.8
C14—C13—S1	119.45 (10)	C36—C35—H35	119.8
C15—C14—C13	118.22 (12)	N31—C36—C35	121.25 (12)
C15—C14—C11	121.46 (12)	N31—C36—C30	116.98 (12)
C13—C14—C11	120.31 (12)	C35—C36—C30	121.73 (11)

C14—C15—C16	119.93 (12)	C36—C30—C37	110.87 (11)
C14—C15—H15	120.0	C36—C30—C38	107.61 (12)
C16—C15—H15	120.0	C37—C30—C38	109.93 (13)
N11—C16—C15	120.92 (12)	C36—C30—C39	110.55 (12)
N11—C16—C10	114.85 (12)	C37—C30—C39	108.74 (13)
C15—C16—C10	124.23 (11)	C38—C30—C39	109.14 (11)
C16—C10—C17	111.42 (12)	C30—C37—H371	109.5
C16—C10—C19	109.56 (11)	C30—C37—H372	109.5
C17—C10—C19	108.90 (11)	H371—C37—H372	109.5
C16—C10—C18	108.38 (11)	C30—C37—H373	109.5
C17—C10—C18	109.27 (12)	H371—C37—H373	109.5
C19—C10—C18	109.29 (13)	H372—C37—H373	109.5
C10—C17—H171	109.5	C30—C38—H381	109.5
C10—C17—H172	109.5	C30—C38—H382	109.5
H171—C17—H172	109.5	H381—C38—H382	109.5
C10—C17—H173	109.5	C30—C38—H383	109.5
H171—C17—H173	109.5	H381—C38—H383	109.5
H172—C17—H173	109.5	H382—C38—H383	109.5
C10—C18—H181	109.5	C30—C39—H391	109.5
C10—C18—H182	109.5	C30—C39—H392	109.5
H181—C18—H182	109.5	H391—C39—H392	109.5
C10—C18—H183	109.5	C30—C39—H393	109.5
H181—C18—H183	109.5	H391—C39—H393	109.5
H182—C18—H183	109.5	H392—C39—H393	109.5
C10—C19—H191	109.5	C34—C31—H311	109.5
C10—C19—H192	109.5	C34—C31—H312	109.5
H191—C19—H192	109.5	H311—C31—H312	109.5
C10—C19—H193	109.5	C34—C31—H313	109.5
H191—C19—H193	109.5	H311—C31—H313	109.5
H192—C19—H193	109.5	H312—C31—H313	109.5
C14—C11—H111	109.5	C51—P1—C61	104.83 (6)
C14—C11—H112	109.5	C51—P1—C41	101.94 (6)
H111—C11—H112	109.5	C61—P1—C41	102.71 (6)
C14—C11—H113	109.5	C41—P1—Cu1	116.97 (5)
H111—C11—H113	109.5	C51—P1—Cu1	112.57 (4)
H112—C11—H113	109.5	C61—P1—Cu1	116.10 (4)
C23—S2—Cu1	109.00 (4)	C46—C41—C42	119.16 (13)
C26—N21—N22	119.20 (11)	C46—C41—P1	118.79 (10)
N21—N22—C23	124.10 (11)	C42—C41—P1	121.92 (11)
N21—N22—B1	113.18 (10)	C43—C42—C41	120.30 (14)
C23—N22—B1	122.68 (11)	C43—C42—H42	119.9
N22—C23—C24	117.34 (12)	C41—C42—H42	119.9
N22—C23—S2	122.08 (10)	C44—C43—C42	120.14 (14)
C24—C23—S2	120.58 (10)	C44—C43—H43	119.9
C25—C24—C23	118.22 (12)	C42—C43—H43	119.9
C25—C24—C21	121.41 (13)	C45—C44—C43	119.93 (14)
C23—C24—C21	120.37 (13)	C45—C44—H44	120.0
C24—C25—C26	120.11 (13)	C43—C44—H44	120.0

C24—C25—H25	119.9	C44—C45—C46	120.19 (14)
C26—C25—H25	119.9	C44—C45—H45	119.9
N21—C26—C25	120.96 (13)	C46—C45—H45	119.9
N21—C26—C70	117.1 (3)	C41—C46—C45	120.26 (13)
C25—C26—C70	120.3 (3)	C41—C46—H46	119.9
N21—C26—C20	113.66 (19)	C45—C46—H46	119.9
C25—C26—C20	125.1 (2)	C52—C51—C56	118.81 (12)
C27—C20—C29	110.2 (4)	C52—C51—P1	117.65 (10)
C27—C20—C28	109.2 (4)	C56—C51—P1	123.46 (10)
C29—C20—C28	108.5 (3)	C53—C52—C51	120.61 (13)
C27—C20—C26	111.3 (4)	C53—C52—H52	119.7
C29—C20—C26	106.0 (3)	C51—C52—H52	119.7
C28—C20—C26	111.6 (3)	C54—C53—C52	119.99 (13)
C20—C27—H271	109.5	C54—C53—H53	120.0
C20—C27—H272	109.5	C52—C53—H53	120.0
H271—C27—H272	109.5	C53—C54—C55	119.90 (13)
C20—C27—H273	109.5	C53—C54—H54	120.1
H271—C27—H273	109.5	C55—C54—H54	120.1
H272—C27—H273	109.5	C56—C55—C54	120.24 (14)
C20—C28—H281	109.5	C56—C55—H55	119.9
C20—C28—H282	109.5	C54—C55—H55	119.9
H281—C28—H282	109.5	C55—C56—C51	120.46 (13)
C20—C28—H283	109.5	C55—C56—H56	119.8
H281—C28—H283	109.5	C51—C56—H56	119.8
H282—C28—H283	109.5	C62—C61—C66	118.86 (13)
C20—C29—H291	109.5	C62—C61—P1	123.09 (11)
C20—C29—H292	109.5	C66—C61—P1	117.90 (11)
H291—C29—H292	109.5	C61—C62—C63	120.57 (15)
C20—C29—H293	109.5	C61—C62—H62	119.7
H291—C29—H293	109.5	C63—C62—H62	119.7
H292—C29—H293	109.5	C64—C63—C62	119.99 (16)
C26—C70—C77	108.1 (4)	C64—C63—H63	120.0
C26—C70—C79	106.6 (7)	C62—C63—H63	120.0
C77—C70—C79	110.4 (8)	C65—C64—C63	120.00 (14)
C26—C70—C78	114.0 (4)	C65—C64—H64	120.0
C77—C70—C78	110.0 (5)	C63—C64—H64	120.0
C79—C70—C78	107.7 (6)	C64—C65—C66	120.18 (14)
C70—C77—H771	109.5	C64—C65—H65	119.9
C70—C77—H772	109.5	C66—C65—H65	119.9
H771—C77—H772	109.5	C65—C66—C61	120.39 (14)
C70—C77—H773	109.5	C65—C66—H66	119.8
H771—C77—H773	109.5	C61—C66—H66	119.8
H772—C77—H773	109.5	Cl81—C8—Cl82	110.31 (8)
C70—C78—H781	109.5	Cl81—C8—Cl83	110.63 (9)
C70—C78—H782	109.5	Cl82—C8—Cl83	110.60 (8)
H781—C78—H782	109.5	Cl81—C8—H8	108.4
C70—C78—H783	109.5	Cl82—C8—H8	108.4
H781—C78—H783	109.5	Cl83—C8—H8	108.4

H782—C78—H783	109.5	Cl91—C9—Cl92	111.44 (9)
C70—C79—H791	109.5	Cl91—C9—Cl93	110.87 (9)
C70—C79—H792	109.5	Cl92—C9—Cl93	110.39 (9)
H791—C79—H792	109.5	Cl91—C9—H9	108.0
C70—C79—H793	109.5	Cl92—C9—H9	108.0
H791—C79—H793	109.5	Cl93—C9—H9	108.0
C16—N11—N12—C13	−4.62 (17)	N22—B1—N32—N31	−114.27 (11)
C16—N11—N12—B1	172.39 (10)	N12—B1—N32—N31	2.42 (15)
N22—B1—N12—N11	47.59 (12)	N22—B1—N32—C33	67.88 (14)
N32—B1—N12—N11	−70.82 (12)	N12—B1—N32—C33	−175.42 (11)
N22—B1—N12—C13	−135.54 (12)	N31—N32—C33—C34	−0.05 (19)
N32—B1—N12—C13	106.06 (13)	B1—N32—C33—C34	177.58 (12)
N11—N12—C13—C14	11.26 (17)	N31—N32—C33—S3	178.70 (10)
B1—N12—C13—C14	−165.23 (11)	B1—N32—C33—S3	−3.66 (17)
N11—N12—C13—S1	−167.35 (9)	N32—C33—C34—C35	1.3 (2)
B1—N12—C13—S1	16.15 (17)	S3—C33—C34—C35	−177.46 (12)
Cu1—S1—C13—N12	15.88 (11)	N32—C33—C34—C31	−178.99 (14)
Cu1—S1—C13—C14	−162.71 (9)	S3—C33—C34—C31	2.3 (2)
N12—C13—C14—C15	−8.97 (17)	C33—C34—C35—C36	−1.5 (2)
S1—C13—C14—C15	169.71 (10)	C31—C34—C35—C36	178.80 (15)
N12—C13—C14—C11	172.44 (11)	N32—N31—C36—C35	0.82 (19)
S1—C13—C14—C11	−8.89 (16)	N32—N31—C36—C30	−177.05 (11)
C13—C14—C15—C16	0.72 (18)	C34—C35—C36—N31	0.4 (2)
C11—C14—C15—C16	179.30 (12)	C34—C35—C36—C30	178.20 (14)
N12—N11—C16—C15	−4.40 (18)	N31—C36—C30—C37	−18.16 (18)
N12—N11—C16—C10	175.23 (10)	C35—C36—C30—C37	163.98 (14)
C14—C15—C16—N11	6.19 (19)	N31—C36—C30—C38	102.08 (14)
C14—C15—C16—C10	−173.40 (12)	C35—C36—C30—C38	−75.78 (16)
N11—C16—C10—C17	174.32 (11)	N31—C36—C30—C39	−138.82 (13)
C15—C16—C10—C17	−6.06 (17)	C35—C36—C30—C39	43.32 (18)
N11—C16—C10—C19	53.75 (15)	C51—P1—C41—C46	−104.71 (11)
C15—C16—C10—C19	−126.63 (14)	C61—P1—C41—C46	146.88 (11)
N11—C16—C10—C18	−65.42 (15)	Cu1—P1—C41—C46	18.51 (12)
C15—C16—C10—C18	114.20 (14)	C51—P1—C41—C42	71.21 (12)
C26—N21—N22—C23	2.59 (19)	C61—P1—C41—C42	−37.20 (12)
C26—N21—N22—B1	−179.56 (12)	Cu1—P1—C41—C42	−165.57 (9)
N32—B1—N22—N21	18.17 (14)	C46—C41—C42—C43	1.0 (2)
N12—B1—N22—N21	−100.99 (11)	P1—C41—C42—C43	−174.91 (10)
N32—B1—N22—C23	−163.94 (11)	C41—C42—C43—C44	−0.3 (2)
N12—B1—N22—C23	76.90 (13)	C42—C43—C44—C45	−0.3 (2)
N21—N22—C23—C24	−1.08 (18)	C43—C44—C45—C46	0.4 (2)
B1—N22—C23—C24	−178.74 (11)	C42—C41—C46—C45	−1.0 (2)
N21—N22—C23—S2	179.14 (9)	P1—C41—C46—C45	175.07 (11)
B1—N22—C23—S2	1.48 (16)	C44—C45—C46—C41	0.3 (2)
Cu1—S2—C23—N22	22.51 (11)	C61—P1—C51—C52	−139.34 (11)
Cu1—S2—C23—C24	−157.27 (10)	C41—P1—C51—C52	113.88 (11)
N22—C23—C24—C25	−1.49 (19)	Cu1—P1—C51—C52	−12.27 (12)

S2—C23—C24—C25	178.29 (11)	C61—P1—C51—C56	43.95 (13)
N22—C23—C24—C21	179.18 (12)	C41—P1—C51—C56	−62.83 (13)
S2—C23—C24—C21	−1.03 (18)	Cu1—P1—C51—C56	171.02 (10)
C23—C24—C25—C26	2.5 (2)	C56—C51—C52—C53	0.3 (2)
C21—C24—C25—C26	−178.14 (14)	P1—C51—C52—C53	−176.58 (11)
N22—N21—C26—C25	−1.4 (2)	C51—C52—C53—C54	−0.7 (2)
N22—N21—C26—C70	−166.8 (3)	C52—C53—C54—C55	0.2 (2)
N22—N21—C26—C20	172.51 (18)	C53—C54—C55—C56	0.6 (2)
C24—C25—C26—N21	−1.1 (2)	C54—C55—C56—C51	−1.0 (2)
C24—C25—C26—C70	163.8 (3)	C52—C51—C56—C55	0.5 (2)
C24—C25—C26—C20	−174.3 (2)	P1—C51—C56—C55	177.20 (12)
N21—C26—C20—C27	−177.8 (4)	C51—P1—C61—C62	23.27 (14)
C25—C26—C20—C27	−4.2 (5)	C41—P1—C61—C62	129.48 (13)
N21—C26—C20—C29	62.3 (3)	Cu1—P1—C61—C62	−101.60 (12)
C25—C26—C20—C29	−124.0 (3)	C51—P1—C61—C66	−161.18 (11)
N21—C26—C20—C28	−55.6 (3)	C41—P1—C61—C66	−54.97 (12)
C25—C26—C20—C28	118.1 (3)	Cu1—P1—C61—C66	73.95 (11)
N21—C26—C70—C77	−26.0 (5)	C66—C61—C62—C63	0.6 (2)
C25—C26—C70—C77	168.5 (4)	P1—C61—C62—C63	176.07 (13)
N21—C26—C70—C79	−144.6 (6)	C61—C62—C63—C64	0.1 (3)
C25—C26—C70—C79	49.9 (7)	C62—C63—C64—C65	−0.6 (3)
N21—C26—C70—C78	96.6 (5)	C63—C64—C65—C66	0.5 (2)
C25—C26—C70—C78	−68.9 (5)	C64—C65—C66—C61	0.2 (2)
C36—N31—N32—C33	−1.01 (19)	C62—C61—C66—C65	−0.7 (2)
C36—N31—N32—B1	−178.73 (11)	P1—C61—C66—C65	−176.45 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···S3^{i}	1.00	2.50	3.4366 (15)	156
C9—H9···S2	1.00	2.68	3.5468 (15)	145
C25—H25···S1^{ii}	0.95	2.70	3.4451 (15)	135
C46—H46···S2	0.95	2.82	3.7480 (15)	164
C66—H66···S3	0.95	2.85	3.7153 (16)	152

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