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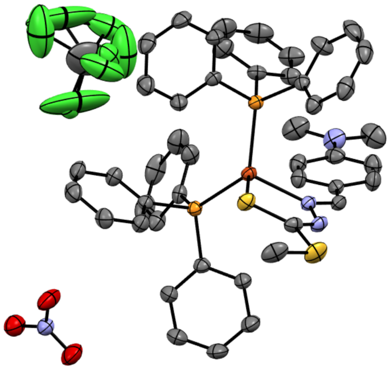

Synthesis and structure of {methyl (*Z*)-2-[4-(dimethylamino)benzylidene]hydrazine-1-carbodithioate-κ^2N^2,S}bis(triphenylphosphine-κP)-copper(I) nitrate carbon tetrachloride monosolvate

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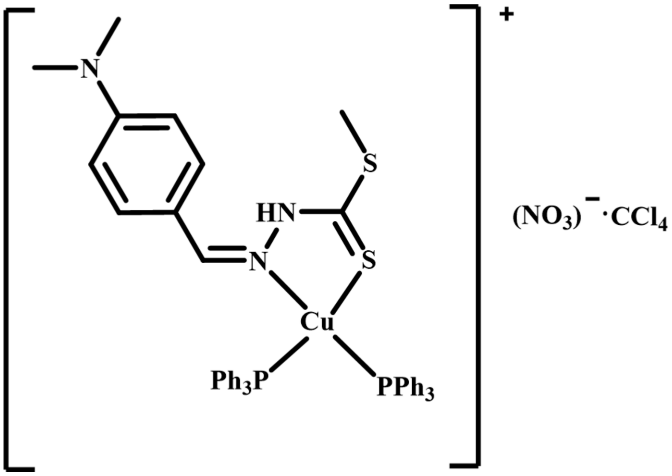
In the title compound, $[Cu(C_{11}H_{15}N_3S_2)\{P(C_6H_5)_3\}_2]NO_3\cdot CCl_4$, the carbon tetrachloride solvent molecule is presumed to have originated as an impurity in the chloroform solvent used. The coordination environment around the copper(I) ion is a distorted $CuNSP_2$ tetrahedron, with a τ_4 structural index of 0.844. In the extended structure, the cation and anion are linked by an N—H$\cdots$O hydrogen bond. Along with electrostatic forces, C—H$\cdots$N, C—H$\cdots$S and C—H$\cdots$O hydrogen bonds help to consolidate the crystal packing.

1. Chemical context

Copper(I) complexes exhibit broad applications across medicinal chemistry (Papazoglou *et al.*, 2014), materials science (Hei & Li, 2021), and catalysis (Egbert *et al.*, 2013). Elucidating their structural features provides valuable insights for the innovative design of further copper(I) complexes, thereby enhancing their structure–activity relationships.



Copper(I) complexes bearing nitrogen and sulfur donor ligands are of significant interest owing to the presence of this metal in the active sites of hydrogenases, carbon monoxide dehydrogenases, and blue copper proteins. Complexes of copper(I) with methyl (*Z*)-2-(4-(dimethylamino)benzylidene) hydrazine-1-carbodithioate ligands and their BSA binding properties have been reported in the literature (Malakar *et al.*, 2023). Such copper(I) species are generally obtained by reacting methyl (*Z*)-2-(4-(dimethylamino)benzylidene)hydrazine-1-carbodithioate or its derivatives with appropriate copper(I) precursors. In this context, the present work reports the synthesis and single-crystal X-ray characterization of the title mononuclear mixed-ligand copper(I) complex $[Cu(C_{11}H_{15}N_3S_2)\{P(C_6H_5)_3\}_2]NO_3{\cdot}CCl_4$ (**I**) or $[Cu(NS)(PPh_3)_2]NO_3{\cdot}CCl_4$, where *NS* denotes the methyl (*Z*)-2-(4-(dimethylamino)benzylidene)hydrazine-1-carbodithioate chelating ligand and PPh_3 represents the triphenylphosphine co-ligand.

2. Structural commentary

Compound (**I**) crystallizes in the monoclinic space group $P2_1/n$, with one cation, one anion and one disordered CCl_4 solvent molecule in the asymmetric unit (Fig. 1). The Cu^I atom is bound to an azomethine nitrogen atom and a sulfur atom from the $C_{11}H_{15}N_3S_2$ ligand, generating a five-membered chelate ring, in addition to phosphorous coordination from two triphenylphosphine ligands. The Cu—N1 bond distance [2.112 (3) Å] is substantially shorter than the Cu—S1 distance [2.3599 (11) Å], which is consistent with previously reported complexes containing analogous donor sets (Malakar *et al.*, 2023). The bite angle of the dithiocarbazate fragment, N1—Cu—S1 [84.80 (10)°], is significantly narrower than the bond angles involving the phosphine donors, P1—Cu—P2 [125.29 (4)°], reflecting trends observed in related Cu^I systems incorporating such coordination motifs (Pathaw *et al.*, 2021). The remaining angles in the coordination sphere, namely N1—Cu—P2 [110.95 (9)°], N1—Cu—P1 [115.78 (8)°], S1—Cu—P2 [109.19 (3)°], and S1—Cu—P1 [101.91 (4)°] lie between these two extremes, reflecting the geometric adjustments required to accommodate different donor atoms and steric constraints around the Cu^I centre. The notably wider P1—Cu—P2 bond angle can be ascribed to the steric bulk and spatial demands of the two triphenylphosphine ligands, as observed in Cu^I complexes containing similar types of phosphine ligands (Messmer & Palenik, 2011). The bite angle of the N2—Cu1—S1 chelate ring is intrinsically constrained by the five-membered dithiocarbazate ring, forcing a much smaller angle than the ideal tetrahedral value. Overall, these angular distortions are a direct consequence of the competing electronic and steric influences within the coordination sphere, leading to the observed deviation from perfect tetrahedral geometry. This is reflected in the four-coordinate structural index (τ_4) of 0.844 [$\tau_4 = (360° - (\alpha + \beta))/141°$] where α and β represent the two predominant θ angles in the four-coordinate complex (Yang *et al.*, 2007): τ_4 is unity and zero for perfect tetrahedral and square planar geometries, respectively).

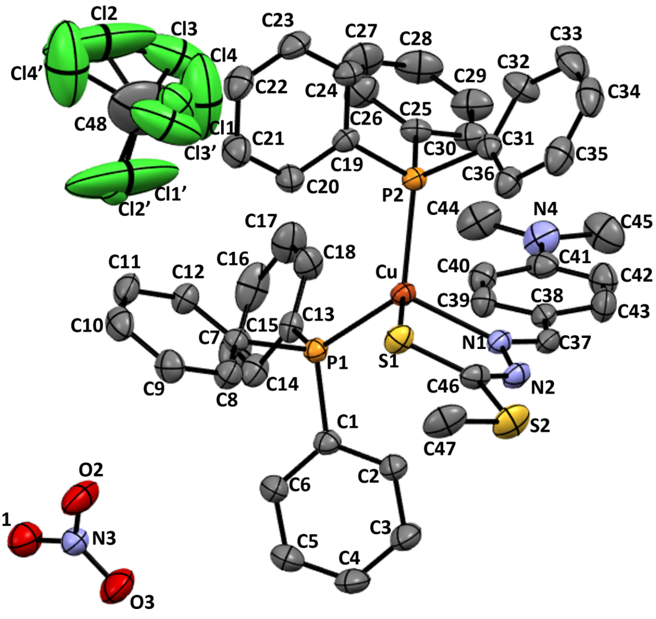


Figure 1
The molecular structure of (**I**) with displacement ellipsoids drawn at the 30% probability level. H atoms are omitted for clarity.

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N2—H2*A*$\cdots$O2^i	0.82	1.96	2.754 (5)	163
C2—H2$\cdots$N1	0.93	2.55	3.391 (5)	151
C36—H36$\cdots$S1	0.93	2.87	3.758 (5)	160
C37—H37$\cdots$O2^i	0.93	2.66	3.384 (5)	135
C47—H47*A*$\cdots$O2	0.96	2.52	3.322 (6)	141

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

Even though (**I**) was synthesized using chloroform, the single-crystal X-ray structure revealed the presence of included carbon tetrachloride (CCl_4) molecules. This can arise as commercial chloroform often contains trace amounts of CCl_4 as a stabilizer or residual impurity from industrial production. These minor amounts of solvate can crystallize during slow evaporation and be incorporated in the crystal. As a result of the weak van der Waals interactions, the CCl_4 molecules occupy voids in the crystal rather than coordinating to the metal centre (Huber *et al.*, 1978).

3. Supramolecular features

In the crystal, an N—H$\cdots$O bond (Table 1) links the cation with the anion. The packing in the extended structure of (**I**) is consolidated by C—H$\cdots$N, C—H$\cdots$S and C—H$\cdots$O interactions. All of the hydrogen-to-acceptor distances are less than 2.9 Å, and the donor-to-acceptor distances are less than 3.5 Å. Moreover, all of the hydrogen-bonding interactions exhibit *D*—H$\cdots$*A* bond angles greater than 130°. The complete interaction details are illustrated in the packing diagram of the compound shown in Fig. 2.

4. Hirshfeld Surface Analysis

Hirshfeld surface analysis was carried out using the *Crystal Explorer 21.5* software package. The surfaces were generated over d_{norm} and two-dimensional fingerprint plots were

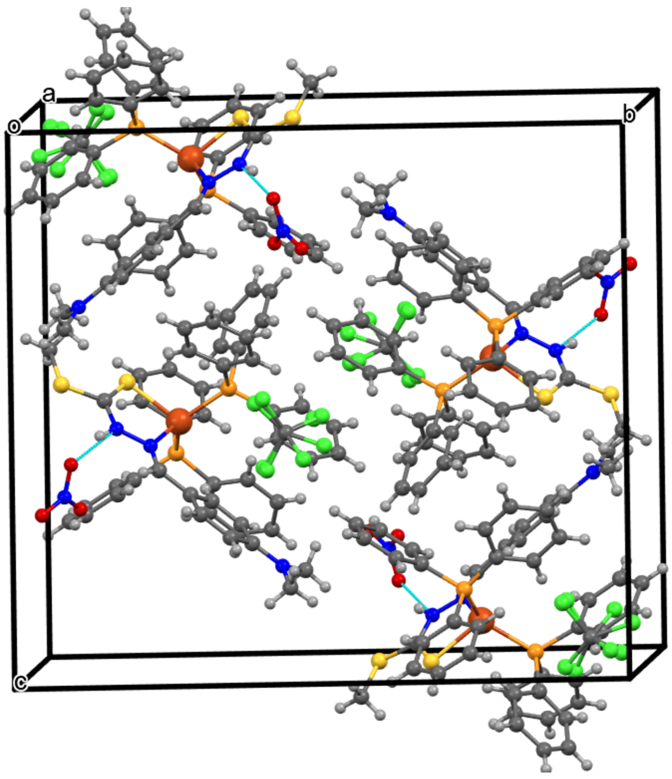
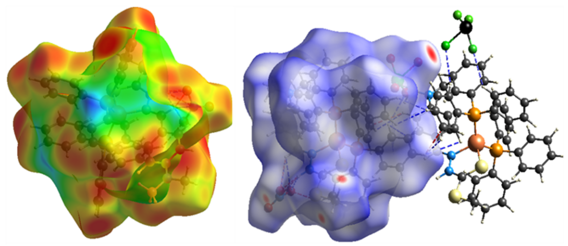


Figure 2
The crystal packing of (**I**) with the N—H···O hydrogen bonds shown as blue dashed lines.

obtained to quantify the directional intermolecular interactions along with other atom-to-atom contacts. Fig. 3(*a*) and (*b*) show the Hirshfeld surfaces mapped over d_i and d_{norm}, respectively. The dark-red spots indicate the presence of close contacts between atoms, while the green regions represent weak contacts. The blue regions, which occupy the majority of the surface, indicate the absence of close contacts in the structure. In Fig. 3(*b*), hydrogen-bond interactions are represented by red dotted lines, whereas other atom-to-atom interactions are represented by blue dotted lines.

According to the two-dimensional fingerprint plots for (**I**) (Fig. 4), the H···H contacts make the largest contribution (61.4%) to the total Hirshfeld surface at a distance range of $d_e + d_i \simeq 1.9$ Å. Similarly, the C···H, O···H, S···H, C···C, N···H, and S···S interactions contribute 9.2%, 5.6%, 2.2%, 1.3%, 0.8%, and 0.4%, respectively.



a) b)

Figure 3
Hirshfeld surfaces for (**I**); (*a*) d_i plot; (*b*) d_{norm} plot.

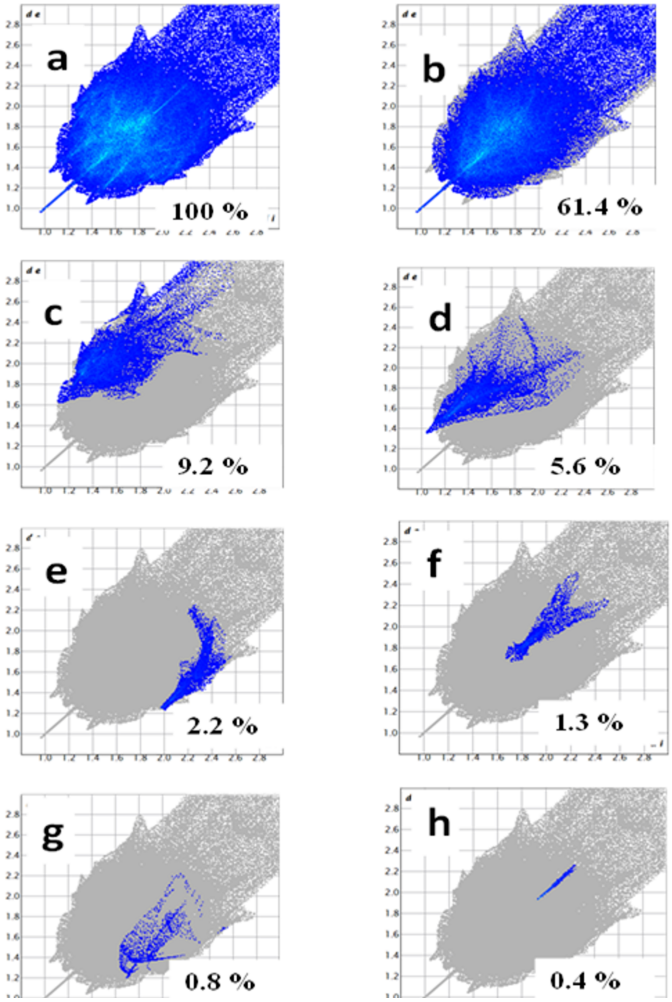


Figure 4
Two-dimensional fingerprint plots for (**I**); (*a*) all interactions and delineated into (*b*) H···H; (*c*) C···H/H···C; (*d*) O···H/H···O; (*e*) S···H/H···S; (*f*) C···C; (*g*) N···H/H···N; (*h*) S···S.

5. Database survey

A SciFinder structure-similarity search for Cu^I complexes bearing *N,S*-bidentate hydrazine-derived carbodithioate ligands in combination with triphenylphosphine donors revealed a small but significant group of structurally related systems. Early studies by Bianchini and co-workers explored the reactivity of bis(triphenylphosphine)copper(I) species toward heterocumulenes such as CO_2, COS, CS_2, and phenyl isothiocyanate, establishing that Cu^I centres supported by phosphines and sulfur-bearing ligands favour distorted tetrahedral coordination and readily engage in S-based bond formation. The Cu—S distances vary from 2.10–2.35 Å for monodentate thiolates to 2.40–2.48 Å in chelating dithiolate environments, while the Cu—P distances lie near 2.27 Å (Bianchini *et al.*, 1983, 2002*a*,*b*). Borate-anchored Cu^I–phosphine complexes were reported by Lobbia *et al.* (1997) in which the Cu atom is coordinated to one phosphine and three pyrazolyl nitrogen atoms in a distorted tetrahedral environment. The N—Cu—P angles fall in the range 120.8 (1)–

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_{11}H_{15}N_3S_2)(C_{18}H_{15}P)_2]NO_3 \cdot CCl_4$
M_r	1057.28
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	10.8364 (18), 22.358 (4), 20.107 (4)
β (°)	98.146 (7)
V (Å^3)	4822.4 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.87
Crystal size (mm)	0.30 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker D8 VENTURE CCD
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.780, 0.845
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	85779, 8478, 6143
R_{int}	0.097
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.168, 1.04
No. of reflections	8478
No. of parameters	590
No. of restraints	52
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.57, −0.91

Computer programs: *APEX3* and *SAINT*), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF*(Westrip, 2010).

130.3 (1)°, and the N—Cu—N angles between 87.5 (1) and 90.8 (1)°, indicating that steric effects from the bulky PCy_3 ligand significantly influence the coordination geometry. Complementary insight into the structural variability of phosphine–supported Cu(I) environments was provided by Bowmaker *et al.* (2002), who characterised three-coordinate tricyclohexylphosphine complexes, which crystallise in several polymorphic forms but maintain Cu—P distances in the 2.20–2.29 Å range and exhibit comparable P—Cu—P angles, and acylpyrazolonate bis(phosphine) derivatives were described by Marchetti *et al.*, (2000) and Eller & Kubas, (2002), who demonstrated that sulfur dioxide binding to Cu^I phosphine thiolate systems stabilizes unusual S- and Se-coordinated adducts, which further expanded the structural space, confirming that phosphine steric effects and ancillary ligand denticity modulate tetrahedral *versus* pseudo-trigonal coordination. The adaptability of Cu^I coordination spheres in the presence of mixed N- and S-donors was additionally illustrated in phenanthroline-containing systems (Mutrofin *et al.*, 2008; Pettinari *et al.*, 1996) who reported phosphine-stabilized Cu^I–pyrazole salts that display diverse supramolecular assemblies through hydrogen-bonding interactions. Across this literature landscape, κ^2-*N,S* chelation in combination with monodentate phosphine donors emerges as a recurring theme. Several copper(I) and copper(II) systems with tricyclohexyl- or triphenylphosphine donors were reported, as well as analogous Ni, Pd, Pt, Ag, and Ru complexes. Notably, nitrate-bound tricyclohexylphosphine copper complexes and thiolate-bridged Cu^I–phosphine derivatives exhibit similar coordination features. However, no previous report describes a Cu^I system incorporating a methyl-substituted (*Z*)-hydrazine-1-carbodithioate ligand combined with triphenylphosphine and nitrate, confirming the novelty of the present structure.

6. Synthesis and crystallization

To a 20 ml chloroform solution of the metal precursor $[Cu(PPh_3)_2NO_3]$ (0.325 g, 0.500 mmol), the ligand methyl (*Z*)-2-(4-(dimethylamino)benzylidene)hydrazine-1-carbodithioate (0.126 g, 0.500 mmol) was added and stirred at room temperature for 12 h. The solution was then evaporated, and the desired complex was precipitated by diethyl ether (40 ml) and dried under vacuum. The obtained product was then recrystallized from chloroform solution by slow evaporation to give yellow needles of (**I**). Yield: 65%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = 1.2–1.5U_{eq}(C)$.

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supporting information

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Synthesis and structure of {methyl (*Z*)-2-[4-(dimethylamino)benzylidene]hydrazine-1-carbodithioate-κ^2N^2,*S*}bis(triphenylphosphine-κP)copper(I) nitrate carbon tetrachloride monosolvate

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Computing details

{Methyl (*Z*)-2-[4-(dimethylamino)benzylidene]hydrazine-1-carbodithioate-κ^2N^2,*S*}bis(triphenylphosphine-κP)copper(I) nitrate carbon tetrachloride monosolvate

Crystal data

$[Cu(C_{11}H_{15}N_3S_2)(C_{18}H_{15}P)_2]NO_3\cdot CCl_4$
$M_r = 1057.28$
Monoclinic, $P2_1/n$
$a = 10.8364$ (18) Å
$b = 22.358$ (4) Å
$c = 20.107$ (4) Å
$\beta = 98.146$ (7)°
$V = 4822.4$ (16) Å^3
$Z = 4$
$F(000) = 2176$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8478 reflections
$\theta = 2.0$–25.0°
$\mu = 0.87$ mm^{-1}
$T = 293$ K
Needle, yellow
0.30 × 0.22 × 0.20 mm

Data collection

Bruker D8 VENTURE CCD diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
$T_{min} = 0.780$, $T_{max} = 0.845$
85779 measured reflections
8478 independent reflections
6143 reflections with $I > 2\sigma(I)$
$R_{int} = 0.097$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -12\rightarrow12$
$k = -26\rightarrow26$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.168$
$S = 1.04$
8478 reflections
590 parameters
52 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0965P)^2 + 2.9941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}
Extinction correction: SHELXL-2019/2 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0013 (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.

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
C1	3.0510 (3)	0.13767 (17)	0.68718 (18)	0.0465 (9)	
C2	2.9398 (4)	0.1173 (2)	0.7063 (2)	0.0553 (10)	
H2	2.867151	0.139233	0.694544	0.066*	
C3	2.9357 (5)	0.0647 (2)	0.7424 (2)	0.0726 (14)	
H3	2.860989	0.051497	0.754977	0.087*	
C4	3.0431 (5)	0.0325 (2)	0.7595 (3)	0.0788 (15)	
H4	3.040878	−0.002617	0.784103	0.095*	
C5	3.1524 (5)	0.0510 (2)	0.7411 (3)	0.0753 (14)	
H5	3.224366	0.028597	0.753176	0.090*	
C6	3.1578 (4)	0.1033 (2)	0.7043 (2)	0.0628 (12)	
H6	3.232832	0.115400	0.691075	0.075*	
C7	3.1742 (3)	0.19743 (17)	0.58957 (18)	0.0427 (9)	
C8	3.1793 (4)	0.1447 (2)	0.5522 (2)	0.0593 (11)	
H8	3.120031	0.114950	0.554549	0.071*	
C9	3.2713 (4)	0.1363 (2)	0.5120 (2)	0.0665 (12)	
H9	3.275139	0.100776	0.488417	0.080*	
C10	3.3567 (4)	0.1805 (3)	0.5071 (2)	0.0707 (13)	
H10	3.418250	0.174973	0.479791	0.085*	
C11	3.3520 (4)	0.2327 (2)	0.5420 (3)	0.0702 (13)	
H11	3.409354	0.262965	0.537876	0.084*	
C12	3.2604 (4)	0.2407 (2)	0.5842 (2)	0.0565 (11)	
H12	3.258766	0.275928	0.608712	0.068*	
C13	3.1098 (3)	0.26363 (19)	0.70024 (19)	0.0485 (10)	
C14	3.1983 (4)	0.2512 (2)	0.7557 (2)	0.0629 (12)	
H14	3.225773	0.212115	0.763530	0.075*	
C15	3.2451 (5)	0.2949 (3)	0.7986 (3)	0.0864 (17)	
H15	3.305382	0.285752	0.834819	0.104*	
C16	3.2045 (6)	0.3521 (4)	0.7888 (3)	0.098 (2)	
H16	3.236378	0.381759	0.818852	0.118*	
C17	3.1166 (5)	0.3669 (3)	0.7349 (3)	0.0907 (18)	
H17	3.089342	0.406184	0.728159	0.109*	
C18	3.0693 (4)	0.3218 (2)	0.6906 (2)	0.0657 (12)	
H18	3.009593	0.331144	0.654129	0.079*	
C19	2.9079 (3)	0.31867 (17)	0.44612 (18)	0.0440 (9)	
C20	3.0136 (4)	0.2842 (2)	0.4469 (2)	0.0606 (12)	
H20	3.032798	0.255689	0.480405	0.073*	
C21	3.0921 (5)	0.2914 (2)	0.3982 (2)	0.0740 (14)	
H21	3.162242	0.267328	0.398696	0.089*	
C22	3.0651 (5)	0.3343 (2)	0.3496 (2)	0.0718 (13)	

H22	3.118750	0.340393	0.317991	0.086*
C23	2.9598 (4)	0.3679 (2)	0.3474 (2)	0.0661 (12)
H23	2.941286	0.396449	0.313889	0.079*
C24	2.8801 (4)	0.35993 (19)	0.3947 (2)	0.0590 (11)
H24	2.807351	0.382426	0.392042	0.071*
C25	2.8157 (4)	0.37910 (17)	0.55577 (19)	0.0492 (10)
C26	2.9089 (5)	0.4208 (2)	0.5522 (3)	0.0719 (13)
H26	2.967071	0.414072	0.523193	0.086*
C27	2.9176 (6)	0.4719 (2)	0.5906 (3)	0.0962 (19)
H27	2.982037	0.498936	0.587929	0.115*
C28	2.8308 (7)	0.4832 (3)	0.6330 (3)	0.098 (2)
H28	2.835634	0.517911	0.658740	0.118*
C29	2.7377 (6)	0.4428 (2)	0.6367 (3)	0.0832 (16)
H29	2.678614	0.450020	0.665011	0.100*
C30	2.7305 (5)	0.3912 (2)	0.5987 (2)	0.0627 (12)
H30	2.666758	0.363976	0.602099	0.075*
C31	2.6534 (3)	0.30880 (18)	0.46096 (18)	0.0467 (9)
C32	2.5847 (5)	0.3598 (2)	0.4473 (3)	0.0778 (15)
H32	2.610620	0.395616	0.468235	0.093*
C33	2.4753 (5)	0.3572 (3)	0.4016 (3)	0.0947 (19)
H33	2.428118	0.391707	0.392422	0.114*
C34	2.4358 (5)	0.3051 (3)	0.3702 (3)	0.0833 (17)
H34	2.363814	0.304342	0.338950	0.100*
C35	2.5023 (5)	0.2553 (3)	0.3849 (2)	0.0790 (15)
H35	2.474493	0.219539	0.364303	0.095*
C36	2.6122 (4)	0.2554 (2)	0.4304 (2)	0.0595 (11)
H36	2.657198	0.220296	0.440074	0.071*
C37	2.6272 (4)	0.20298 (18)	0.6466 (2)	0.0503 (10)
H37	2.553203	0.181747	0.645880	0.060*
C38	2.6472 (3)	0.25264 (19)	0.69251 (19)	0.0491 (10)
C39	2.7613 (4)	0.28038 (19)	0.7111 (2)	0.0540 (10)
H39	2.830430	0.266560	0.693121	0.065*
C40	2.7754 (4)	0.3271 (2)	0.7548 (2)	0.0591 (11)
H40	2.853898	0.344107	0.766161	0.071*
C41	2.6747 (4)	0.3504 (2)	0.7831 (2)	0.0616 (11)
C42	2.5603 (4)	0.3218 (2)	0.7659 (3)	0.0718 (13)
H42	2.491220	0.335163	0.784262	0.086*
C43	2.5479 (4)	0.2746 (2)	0.7227 (3)	0.0689 (13)
H43	2.470375	0.256280	0.712970	0.083*
C44	2.8032 (6)	0.4290 (3)	0.8405 (3)	0.0986 (19)
H44A	2.794740	0.461341	0.870926	0.148*
H44B	2.865745	0.401674	0.860798	0.148*
H44C	2.827278	0.444588	0.799718	0.148*
C45	2.5846 (6)	0.4168 (3)	0.8588 (3)	0.1000 (19)
H45A	2.608369	0.450975	0.886641	0.150*
H45B	2.514892	0.427070	0.825787	0.150*
H45C	2.561684	0.384591	0.886145	0.150*
C46	2.7232 (4)	0.11030 (17)	0.5255 (2)	0.0520 (10)

C47	2.7519 (6)	0.0203 (2)	0.4333 (3)	0.0858 (17)	
H47A	2.719630	−0.015909	0.411752	0.129*	
H47B	2.756371	0.050690	0.400056	0.129*	
H47C	2.833672	0.012977	0.457141	0.129*	
C48	3.3194 (9)	0.4272 (3)	0.5651 (4)	0.226 (6)	
N1	2.7024 (3)	0.18535 (14)	0.60652 (16)	0.0451 (8)	
N2	2.6641 (3)	0.13278 (15)	0.57286 (17)	0.0515 (8)	
H2A	2.612437	0.108611	0.582327	0.077*	
N3	3.5183 (3)	0.05500 (16)	0.68568 (19)	0.0572 (9)	
N4	2.6876 (4)	0.3986 (2)	0.8257 (2)	0.0806 (12)	
O1	3.6175 (3)	0.07496 (16)	0.71350 (18)	0.0825 (10)	
O2	3.4847 (3)	0.06823 (18)	0.62581 (19)	0.0957 (13)	
O3	3.4555 (4)	0.02164 (18)	0.71447 (19)	0.0932 (12)	
P1	3.04707 (8)	0.20709 (4)	0.63954 (5)	0.0408 (2)	
P2	2.80883 (9)	0.30789 (4)	0.51150 (5)	0.0408 (3)	
S1	2.84891 (10)	0.14034 (5)	0.49953 (5)	0.0546 (3)	
S2	2.65109 (13)	0.04460 (6)	0.49112 (7)	0.0821 (4)	
Cu	2.86077 (4)	0.22336 (2)	0.57262 (2)	0.04075 (17)	
Cl1	3.2286 (4)	0.39592 (19)	0.4997 (3)	0.1015 (9)	0.5
Cl1′	3.4001 (3)	0.3864 (2)	0.6323 (2)	0.1015 (9)	0.5
Cl2	3.4040 (14)	0.4819 (4)	0.5416 (7)	0.360 (7)	0.5
Cl2′	3.3799 (15)	0.3925 (4)	0.6356 (6)	0.360 (7)	0.5
Cl3	3.2687 (9)	0.4928 (3)	0.5874 (4)	0.215 (3)	0.5
Cl3′	3.2528 (9)	0.3816 (3)	0.5083 (4)	0.215 (3)	0.5
Cl4	3.2245 (9)	0.4611 (8)	0.6087 (8)	0.380 (7)	0.5
Cl4′	3.4426 (10)	0.4662 (7)	0.5482 (10)	0.380 (7)	0.5

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.051 (2)	0.049 (2)	0.040 (2)	−0.0006 (18)	0.0054 (16)	0.0050 (17)
C2	0.051 (2)	0.060 (3)	0.055 (2)	0.000 (2)	0.0083 (19)	0.013 (2)
C3	0.069 (3)	0.077 (3)	0.072 (3)	−0.011 (3)	0.011 (2)	0.029 (3)
C4	0.083 (3)	0.070 (3)	0.082 (4)	−0.003 (3)	0.005 (3)	0.036 (3)
C5	0.070 (3)	0.070 (3)	0.084 (3)	0.014 (3)	0.001 (3)	0.026 (3)
C6	0.053 (2)	0.066 (3)	0.070 (3)	0.005 (2)	0.010 (2)	0.017 (2)
C7	0.0407 (19)	0.046 (2)	0.040 (2)	0.0007 (16)	0.0028 (15)	0.0044 (17)
C8	0.058 (2)	0.059 (3)	0.063 (3)	−0.006 (2)	0.016 (2)	−0.002 (2)
C9	0.069 (3)	0.069 (3)	0.066 (3)	0.011 (2)	0.025 (2)	−0.007 (2)
C10	0.061 (3)	0.095 (4)	0.060 (3)	0.011 (3)	0.025 (2)	0.005 (3)
C11	0.054 (3)	0.086 (4)	0.074 (3)	−0.015 (2)	0.020 (2)	0.011 (3)
C12	0.053 (2)	0.059 (3)	0.059 (3)	−0.008 (2)	0.012 (2)	−0.001 (2)
C13	0.0402 (19)	0.061 (3)	0.045 (2)	−0.0083 (18)	0.0096 (17)	−0.0076 (19)
C14	0.057 (2)	0.082 (3)	0.048 (2)	−0.016 (2)	0.001 (2)	−0.001 (2)
C15	0.076 (3)	0.129 (5)	0.052 (3)	−0.033 (4)	0.002 (2)	−0.015 (3)
C16	0.088 (4)	0.131 (6)	0.077 (4)	−0.050 (4)	0.016 (3)	−0.054 (4)
C17	0.089 (4)	0.073 (4)	0.113 (5)	−0.019 (3)	0.024 (4)	−0.037 (3)
C18	0.059 (3)	0.057 (3)	0.078 (3)	−0.010 (2)	0.001 (2)	−0.016 (2)

C19	0.048 (2)	0.042 (2)	0.042 (2)	−0.0087 (17)	0.0058 (16)	0.0003 (17)
C20	0.054 (2)	0.074 (3)	0.055 (3)	0.005 (2)	0.009 (2)	0.015 (2)
C21	0.063 (3)	0.095 (4)	0.068 (3)	0.008 (3)	0.021 (2)	0.009 (3)
C22	0.070 (3)	0.095 (4)	0.054 (3)	−0.012 (3)	0.023 (2)	0.005 (3)
C23	0.078 (3)	0.069 (3)	0.052 (3)	−0.012 (3)	0.013 (2)	0.017 (2)
C24	0.066 (3)	0.057 (3)	0.055 (3)	0.003 (2)	0.012 (2)	0.016 (2)
C25	0.063 (2)	0.039 (2)	0.044 (2)	0.0020 (18)	0.0031 (19)	0.0011 (17)
C26	0.085 (3)	0.057 (3)	0.075 (3)	−0.014 (2)	0.017 (3)	−0.012 (2)
C27	0.116 (5)	0.061 (4)	0.110 (5)	−0.030 (3)	0.009 (4)	−0.021 (3)
C28	0.155 (6)	0.056 (4)	0.078 (4)	0.001 (4)	−0.001 (4)	−0.018 (3)
C29	0.127 (5)	0.066 (4)	0.062 (3)	0.017 (3)	0.027 (3)	−0.004 (3)
C30	0.083 (3)	0.052 (3)	0.055 (3)	0.006 (2)	0.018 (2)	−0.001 (2)
C31	0.042 (2)	0.060 (3)	0.039 (2)	0.0004 (18)	0.0079 (16)	0.0065 (19)
C32	0.078 (3)	0.076 (4)	0.074 (3)	0.018 (3)	−0.009 (3)	0.005 (3)
C33	0.072 (3)	0.123 (5)	0.083 (4)	0.035 (3)	−0.009 (3)	0.022 (4)
C34	0.049 (3)	0.139 (6)	0.059 (3)	−0.002 (3)	−0.001 (2)	0.012 (3)
C35	0.064 (3)	0.113 (5)	0.058 (3)	−0.027 (3)	0.000 (2)	−0.005 (3)
C36	0.054 (2)	0.070 (3)	0.052 (2)	−0.013 (2)	0.0005 (19)	0.000 (2)
C37	0.044 (2)	0.050 (2)	0.057 (2)	−0.0090 (18)	0.0055 (19)	0.013 (2)
C38	0.047 (2)	0.052 (2)	0.050 (2)	0.0038 (19)	0.0126 (18)	0.012 (2)
C39	0.047 (2)	0.063 (3)	0.054 (2)	−0.0023 (19)	0.0130 (19)	−0.002 (2)
C40	0.058 (3)	0.067 (3)	0.053 (3)	−0.008 (2)	0.010 (2)	−0.001 (2)
C41	0.077 (3)	0.059 (3)	0.051 (3)	0.008 (2)	0.018 (2)	0.009 (2)
C42	0.064 (3)	0.081 (4)	0.076 (3)	0.011 (3)	0.026 (2)	−0.004 (3)
C43	0.048 (2)	0.081 (4)	0.080 (3)	−0.004 (2)	0.021 (2)	−0.001 (3)
C44	0.144 (6)	0.082 (4)	0.074 (4)	−0.021 (4)	0.029 (4)	−0.016 (3)
C45	0.116 (5)	0.107 (5)	0.079 (4)	0.029 (4)	0.020 (3)	−0.019 (3)
C46	0.058 (2)	0.039 (2)	0.053 (2)	−0.0109 (18)	−0.012 (2)	0.0025 (18)
C47	0.134 (5)	0.054 (3)	0.069 (3)	−0.031 (3)	0.013 (3)	−0.015 (2)
C48	0.276 (14)	0.118 (8)	0.269 (14)	−0.057 (9)	−0.022 (12)	−0.039 (9)
N1	0.0427 (17)	0.0447 (19)	0.0464 (18)	−0.0082 (14)	0.0007 (14)	0.0075 (15)
N2	0.0520 (19)	0.045 (2)	0.056 (2)	−0.0173 (15)	0.0019 (16)	0.0032 (16)
N3	0.058 (2)	0.054 (2)	0.061 (2)	−0.0015 (18)	0.0158 (19)	0.0054 (18)
N4	0.100 (3)	0.074 (3)	0.073 (3)	−0.001 (2)	0.030 (2)	−0.013 (2)
O1	0.078 (2)	0.088 (3)	0.078 (2)	−0.0154 (19)	−0.0019 (18)	0.0061 (19)
O2	0.091 (2)	0.112 (3)	0.077 (2)	−0.051 (2)	−0.013 (2)	0.030 (2)
O3	0.091 (2)	0.104 (3)	0.090 (3)	−0.022 (2)	0.032 (2)	0.021 (2)
P1	0.0396 (5)	0.0427 (6)	0.0395 (5)	−0.0033 (4)	0.0035 (4)	0.0016 (4)
P2	0.0437 (5)	0.0386 (6)	0.0397 (5)	−0.0037 (4)	0.0044 (4)	0.0024 (4)
S1	0.0611 (6)	0.0450 (6)	0.0580 (6)	−0.0121 (5)	0.0096 (5)	−0.0105 (5)
S2	0.0927 (9)	0.0565 (8)	0.0950 (10)	−0.0351 (7)	0.0060 (8)	−0.0151 (7)
Cu	0.0427 (3)	0.0374 (3)	0.0413 (3)	−0.00711 (19)	0.00314 (19)	0.00170 (19)
Cl1	0.0810 (13)	0.091 (2)	0.125 (2)	−0.0002 (12)	−0.0107 (13)	−0.0179 (16)
Cl1′	0.0810 (13)	0.091 (2)	0.125 (2)	−0.0002 (12)	−0.0107 (13)	−0.0179 (16)
Cl2	0.654 (18)	0.123 (4)	0.265 (8)	−0.131 (7)	−0.071 (9)	0.054 (5)
Cl2′	0.654 (18)	0.123 (4)	0.265 (8)	−0.131 (7)	−0.071 (9)	0.054 (5)
Cl3	0.307 (7)	0.114 (3)	0.190 (4)	0.064 (3)	−0.088 (4)	−0.027 (3)
Cl3′	0.307 (7)	0.114 (3)	0.190 (4)	0.064 (3)	−0.088 (4)	−0.027 (3)

Cl4	0.179 (5)	0.483 (15)	0.499 (16)	−0.046 (7)	0.113 (7)	−0.183 (13)
Cl4′	0.179 (5)	0.483 (15)	0.499 (16)	−0.046 (7)	0.113 (7)	−0.183 (13)

Geometric parameters (Å, º)

C1—C6	1.391 (6)	C30—H30	0.9300
C1—C2	1.392 (5)	C31—C32	1.367 (6)
C1—P1	1.821 (4)	C31—C36	1.387 (6)
C2—C3	1.386 (6)	C31—P2	1.840 (4)
C2—H2	0.9300	C32—C33	1.395 (7)
C3—C4	1.370 (7)	C32—H32	0.9300
C3—H3	0.9300	C33—C34	1.364 (8)
C4—C5	1.356 (7)	C33—H33	0.9300
C4—H4	0.9300	C34—C35	1.338 (8)
C5—C6	1.390 (6)	C34—H34	0.9300
C5—H5	0.9300	C35—C36	1.395 (6)
C6—H6	0.9300	C35—H35	0.9300
C7—C12	1.360 (6)	C36—H36	0.9300
C7—C8	1.404 (6)	C37—N1	1.287 (5)
C7—P1	1.830 (4)	C37—C38	1.440 (6)
C8—C9	1.382 (6)	C37—H37	0.9300
C8—H8	0.9300	C38—C39	1.386 (5)
C9—C10	1.365 (7)	C38—C43	1.398 (6)
C9—H9	0.9300	C39—C40	1.360 (6)
C10—C11	1.369 (7)	C39—H39	0.9300
C10—H10	0.9300	C40—C41	1.400 (6)
C11—C12	1.405 (6)	C40—H40	0.9300
C11—H11	0.9300	C41—N4	1.372 (6)
C12—H12	0.9300	C41—C42	1.395 (7)
C13—C18	1.379 (6)	C42—C43	1.360 (7)
C13—C14	1.392 (5)	C42—H42	0.9300
C13—P1	1.821 (4)	C43—H43	0.9300
C14—C15	1.352 (7)	C44—N4	1.419 (7)
C14—H14	0.9300	C44—H44A	0.9600
C15—C16	1.359 (9)	C44—H44B	0.9600
C15—H15	0.9300	C44—H44C	0.9600
C16—C17	1.378 (9)	C45—N4	1.438 (7)
C16—H16	0.9300	C45—H45A	0.9600
C17—C18	1.393 (7)	C45—H45B	0.9600
C17—H17	0.9300	C45—H45C	0.9600
C18—H18	0.9300	C46—N2	1.320 (5)
C19—C20	1.378 (6)	C46—S1	1.668 (4)
C19—C24	1.386 (5)	C46—S2	1.759 (4)
C19—P2	1.827 (4)	C47—S2	1.788 (6)
C20—C21	1.395 (6)	C47—H47A	0.9600
C20—H20	0.9300	C47—H47B	0.9600
C21—C22	1.370 (7)	C47—H47C	0.9600
C21—H21	0.9300	C48—Cl3′	1.622 (8)

C22—C23	1.362 (7)	C48—Cl4	1.630 (10)
C22—H22	0.9300	C48—Cl2	1.639 (11)
C23—C24	1.384 (6)	C48—Cl3	1.652 (10)
C23—H23	0.9300	C48—Cl2′	1.665 (10)
C24—H24	0.9300	C48—Cl4′	1.670 (10)
C25—C30	1.376 (6)	C48—Cl1	1.680 (8)
C25—C26	1.384 (6)	C48—Cl1′	1.757 (9)
C25—P2	1.821 (4)	N1—N2	1.390 (4)
C26—C27	1.375 (7)	N1—Cu	2.112 (3)
C26—H26	0.9300	N2—H2A	0.8200
C27—C28	1.380 (9)	N3—O3	1.211 (5)
C27—H27	0.9300	N3—O1	1.223 (4)
C28—C29	1.365 (8)	N3—O2	1.243 (5)
C28—H28	0.9300	P1—Cu	2.2911 (10)
C29—C30	1.380 (7)	P2—Cu	2.2808 (11)
C29—H29	0.9300	S1—Cu	2.3599 (11)

C6—C1—C2	118.3 (4)	C31—C32—C33	119.0 (5)
C6—C1—P1	123.8 (3)	C31—C32—H32	120.5
C2—C1—P1	117.9 (3)	C33—C32—H32	120.5
C3—C2—C1	121.1 (4)	C34—C33—C32	121.5 (5)
C3—C2—H2	119.5	C34—C33—H33	119.3
C1—C2—H2	119.5	C32—C33—H33	119.3
C4—C3—C2	119.2 (4)	C35—C34—C33	119.0 (5)
C4—C3—H3	120.4	C35—C34—H34	120.5
C2—C3—H3	120.4	C33—C34—H34	120.5
C5—C4—C3	121.0 (4)	C34—C35—C36	121.7 (5)
C5—C4—H4	119.5	C34—C35—H35	119.1
C3—C4—H4	119.5	C36—C35—H35	119.1
C4—C5—C6	120.5 (4)	C31—C36—C35	118.9 (5)
C4—C5—H5	119.8	C31—C36—H36	120.5
C6—C5—H5	119.8	C35—C36—H36	120.5
C5—C6—C1	120.0 (4)	N1—C37—C38	125.9 (4)
C5—C6—H6	120.0	N1—C37—H37	117.1
C1—C6—H6	120.0	C38—C37—H37	117.1
C12—C7—C8	118.5 (4)	C39—C38—C43	115.9 (4)
C12—C7—P1	122.6 (3)	C39—C38—C37	124.4 (4)
C8—C7—P1	118.9 (3)	C43—C38—C37	119.6 (4)
C9—C8—C7	120.8 (4)	C40—C39—C38	122.2 (4)
C9—C8—H8	119.6	C40—C39—H39	118.9
C7—C8—H8	119.6	C38—C39—H39	118.9
C10—C9—C8	119.8 (5)	C39—C40—C41	121.7 (4)
C10—C9—H9	120.1	C39—C40—H40	119.2
C8—C9—H9	120.1	C41—C40—H40	119.2
C9—C10—C11	120.3 (4)	N4—C41—C42	121.6 (4)
C9—C10—H10	119.8	N4—C41—C40	121.9 (5)
C11—C10—H10	119.8	C42—C41—C40	116.5 (4)
C10—C11—C12	120.0 (4)	C43—C42—C41	121.2 (4)

C10—C11—H11	120.0	C43—C42—H42	119.4
C12—C11—H11	120.0	C41—C42—H42	119.4
C7—C12—C11	120.6 (4)	C42—C43—C38	122.5 (4)
C7—C12—H12	119.7	C42—C43—H43	118.8
C11—C12—H12	119.7	C38—C43—H43	118.8
C18—C13—C14	118.0 (4)	N4—C44—H44A	109.5
C18—C13—P1	118.7 (3)	N4—C44—H44B	109.5
C14—C13—P1	123.3 (4)	H44A—C44—H44B	109.5
C15—C14—C13	121.3 (5)	N4—C44—H44C	109.5
C15—C14—H14	119.3	H44A—C44—H44C	109.5
C13—C14—H14	119.3	H44B—C44—H44C	109.5
C14—C15—C16	120.2 (5)	N4—C45—H45A	109.5
C14—C15—H15	119.9	N4—C45—H45B	109.5
C16—C15—H15	119.9	H45A—C45—H45B	109.5
C15—C16—C17	120.9 (5)	N4—C45—H45C	109.5
C15—C16—H16	119.5	H45A—C45—H45C	109.5
C17—C16—H16	119.5	H45B—C45—H45C	109.5
C16—C17—C18	118.7 (6)	N2—C46—S1	125.0 (3)
C16—C17—H17	120.7	N2—C46—S2	111.6 (3)
C18—C17—H17	120.7	S1—C46—S2	123.4 (3)
C13—C18—C17	120.8 (5)	S2—C47—H47A	109.5
C13—C18—H18	119.6	S2—C47—H47B	109.5
C17—C18—H18	119.6	H47A—C47—H47B	109.5
C20—C19—C24	118.2 (4)	S2—C47—H47C	109.5
C20—C19—P2	119.4 (3)	H47A—C47—H47C	109.5
C24—C19—P2	122.4 (3)	H47B—C47—H47C	109.5
C19—C20—C21	121.1 (4)	Cl3′—C48—Cl3	128.2 (7)
C19—C20—H20	119.4	Cl2—C48—Cl2′	115.1 (8)
C21—C20—H20	119.4	Cl4—C48—Cl4′	116.8 (9)
C22—C21—C20	119.4 (5)	Cl1—C48—Cl1′	124.0 (5)
C22—C21—H21	120.3	C37—N1—N2	113.1 (3)
C20—C21—H21	120.3	C37—N1—Cu	134.0 (3)
C23—C22—C21	120.1 (4)	N2—N1—Cu	112.5 (2)
C23—C22—H22	119.9	C46—N2—N1	122.1 (3)
C21—C22—H22	119.9	C46—N2—H2A	109.5
C22—C23—C24	120.6 (4)	N1—N2—H2A	127.7
C22—C23—H23	119.7	O3—N3—O1	121.5 (4)
C24—C23—H23	119.7	O3—N3—O2	120.1 (4)
C23—C24—C19	120.4 (4)	O1—N3—O2	118.3 (4)
C23—C24—H24	119.8	C41—N4—C44	121.1 (4)
C19—C24—H24	119.8	C41—N4—C45	119.7 (5)
C30—C25—C26	117.4 (4)	C44—N4—C45	119.2 (5)
C30—C25—P2	119.5 (3)	C13—P1—C1	105.10 (18)
C26—C25—P2	122.9 (3)	C13—P1—C7	102.20 (17)
C27—C26—C25	121.6 (5)	C1—P1—C7	103.01 (18)
C27—C26—H26	119.2	C13—P1—Cu	119.84 (14)
C25—C26—H26	119.2	C1—P1—Cu	113.40 (12)
C26—C27—C28	120.0 (6)	C7—P1—Cu	111.46 (12)

C26—C27—H27	120.0	C25—P2—C19	104.41 (18)
C28—C27—H27	120.0	C25—P2—C31	103.36 (18)
C29—C28—C27	119.1 (5)	C19—P2—C31	100.75 (17)
C29—C28—H28	120.4	C25—P2—Cu	118.12 (13)
C27—C28—H28	120.4	C19—P2—Cu	111.82 (13)
C28—C29—C30	120.6 (5)	C31—P2—Cu	116.33 (13)
C28—C29—H29	119.7	C46—S1—Cu	95.54 (16)
C30—C29—H29	119.7	C46—S2—C47	103.4 (2)
C25—C30—C29	121.4 (5)	N1—Cu—P2	110.95 (9)
C25—C30—H30	119.3	N1—Cu—P1	115.78 (8)
C29—C30—H30	119.3	P2—Cu—P1	125.29 (4)
C32—C31—C36	119.8 (4)	N1—Cu—S1	84.80 (10)
C32—C31—P2	123.3 (3)	P2—Cu—S1	109.19 (4)
C36—C31—P2	116.5 (3)	P1—Cu—S1	101.91 (4)

C6—C1—C2—C3	1.2 (6)	N4—C41—C42—C43	178.9 (5)
P1—C1—C2—C3	179.8 (4)	C40—C41—C42—C43	−1.3 (7)
C1—C2—C3—C4	−0.1 (7)	C41—C42—C43—C38	−0.9 (8)
C2—C3—C4—C5	−0.5 (8)	C39—C38—C43—C42	2.4 (7)
C3—C4—C5—C6	−0.1 (9)	C37—C38—C43—C42	−179.2 (4)
C4—C5—C6—C1	1.2 (8)	C38—C37—N1—N2	174.1 (3)
C2—C1—C6—C5	−1.8 (7)	C38—C37—N1—Cu	−13.9 (6)
P1—C1—C6—C5	179.7 (4)	S1—C46—N2—N1	0.1 (5)
C12—C7—C8—C9	1.3 (6)	S2—C46—N2—N1	−178.8 (2)
P1—C7—C8—C9	177.8 (3)	C37—N1—N2—C46	174.2 (3)
C7—C8—C9—C10	−1.7 (7)	Cu—N1—N2—C46	0.4 (4)
C8—C9—C10—C11	0.4 (7)	C42—C41—N4—C44	−177.2 (5)
C9—C10—C11—C12	1.2 (7)	C40—C41—N4—C44	3.0 (7)
C8—C7—C12—C11	0.2 (6)	C42—C41—N4—C45	6.2 (7)
P1—C7—C12—C11	−176.1 (3)	C40—C41—N4—C45	−173.5 (5)
C10—C11—C12—C7	−1.5 (7)	C18—C13—P1—C1	−150.4 (3)
C18—C13—C14—C15	−1.1 (7)	C14—C13—P1—C1	30.4 (4)
P1—C13—C14—C15	178.0 (4)	C18—C13—P1—C7	102.3 (4)
C13—C14—C15—C16	1.3 (8)	C14—C13—P1—C7	−76.8 (4)
C14—C15—C16—C17	−0.9 (9)	C18—C13—P1—Cu	−21.5 (4)
C15—C16—C17—C18	0.4 (9)	C14—C13—P1—Cu	159.4 (3)
C14—C13—C18—C17	0.6 (7)	C6—C1—P1—C13	−79.5 (4)
P1—C13—C18—C17	−178.6 (4)	C2—C1—P1—C13	101.9 (3)
C16—C17—C18—C13	−0.3 (8)	C6—C1—P1—C7	27.2 (4)
C24—C19—C20—C21	1.4 (6)	C2—C1—P1—C7	−151.4 (3)
P2—C19—C20—C21	−179.5 (4)	C6—C1—P1—Cu	147.8 (3)
C19—C20—C21—C22	1.3 (7)	C2—C1—P1—Cu	−30.8 (4)
C20—C21—C22—C23	−2.5 (8)	C12—C7—P1—C13	−24.3 (4)
C21—C22—C23—C24	1.0 (8)	C8—C7—P1—C13	159.3 (3)
C22—C23—C24—C19	1.7 (7)	C12—C7—P1—C1	−133.2 (3)
C20—C19—C24—C23	−2.9 (6)	C8—C7—P1—C1	50.5 (3)
P2—C19—C24—C23	178.0 (3)	C12—C7—P1—Cu	104.9 (3)
C30—C25—C26—C27	0.9 (7)	C8—C7—P1—Cu	−71.5 (3)

P2—C25—C26—C27	−174.5 (4)	C30—C25—P2—C19	165.8 (3)
C25—C26—C27—C28	−1.2 (9)	C26—C25—P2—C19	−19.0 (4)
C26—C27—C28—C29	0.7 (10)	C30—C25—P2—C31	60.8 (4)
C27—C28—C29—C30	0.2 (9)	C26—C25—P2—C31	−124.0 (4)
C26—C25—C30—C29	0.0 (7)	C30—C25—P2—Cu	−69.3 (4)
P2—C25—C30—C29	175.5 (4)	C26—C25—P2—Cu	106.0 (4)
C28—C29—C30—C25	−0.5 (8)	C20—C19—P2—C25	117.1 (3)
C36—C31—C32—C33	−1.3 (7)	C24—C19—P2—C25	−63.8 (4)
P2—C31—C32—C33	171.9 (4)	C20—C19—P2—C31	−135.9 (3)
C31—C32—C33—C34	−0.3 (9)	C24—C19—P2—C31	43.2 (4)
C32—C33—C34—C35	1.7 (9)	C20—C19—P2—Cu	−11.7 (4)
C33—C34—C35—C36	−1.5 (8)	C24—C19—P2—Cu	167.4 (3)
C32—C31—C36—C35	1.5 (6)	C32—C31—P2—C25	17.6 (4)
P2—C31—C36—C35	−172.1 (3)	C36—C31—P2—C25	−169.0 (3)
C34—C35—C36—C31	−0.1 (7)	C32—C31—P2—C19	−90.1 (4)
N1—C37—C38—C39	−15.1 (6)	C36—C31—P2—C19	83.2 (3)
N1—C37—C38—C43	166.7 (4)	C32—C31—P2—Cu	148.8 (4)
C43—C38—C39—C40	−1.6 (6)	C36—C31—P2—Cu	−37.8 (3)
C37—C38—C39—C40	−179.9 (4)	N2—C46—S1—Cu	−0.5 (4)
C38—C39—C40—C41	−0.6 (7)	S2—C46—S1—Cu	178.3 (2)
C39—C40—C41—N4	−178.1 (4)	N2—C46—S2—C47	−176.3 (3)
C39—C40—C41—C42	2.1 (7)	S1—C46—S2—C47	4.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.82	1.96	2.754 (5)	163
C2—H2···N1	0.93	2.55	3.391 (5)	151
C36—H36···S1	0.93	2.87	3.758 (5)	160
C37—H37···O2^{i}	0.93	2.66	3.384 (5)	135
C47—H47*A*···O2	0.96	2.52	3.322 (6)	141

Symmetry code: (i) *x*−1, *y*, *z*.