



μ_3 -Chlorido- μ_2 -chlorido-(μ_3 -pyrrolidine-1-carbo-dithioato- κ^4 S:S,S':S')tris[(triethylphosphane- κ P)-copper(I)]: crystal structure and Hirshfeld surface analysis

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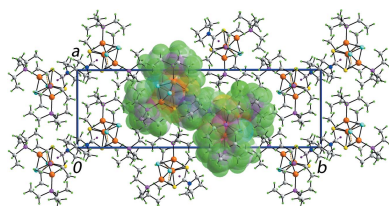
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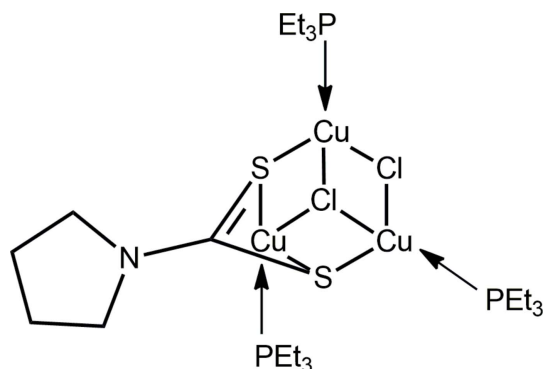
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The title trinuclear compound, [Cu₃(C₅H₈NS₂)Cl₂(C₆H₁₅P)₃], has the dithiocarbamate ligand symmetrically chelating one Cu^I atom and each of the S atoms bridging to another Cu^I atom. Both chloride ligands are bridging, one being μ_3 - and the other μ_2 -bridging. Each Et₃P ligand occupies a terminal position. Two of the Cu^I atoms exist within Cl₂PS donor sets and the third is based on a CIPS₂ donor set, with each coordination geometry based on a distorted tetrahedron. The constituents defining the core of the molecule, *i.e.* Cu₃Cl₂S₂, occupy seven corners of a distorted cube. In the crystal, linear supramolecular chains along the *c* axis are formed *via* phosphane–methylene–C–H...Cl and pyrrolidine–methylene–C–H... π (chelate) interactions, and these chains pack without directional interactions between them. An analysis of the Hirshfeld surface points to the predominance of H atoms at the surface, *i.e.* contributing 86.6% to the surface, and also highlights the presence of C–H... π (chelate) interactions.

1. Chemical context

Recent studies have highlighted the potential of ternary coinage metal phosphane/dithiocarbamates as anti-microbial agents. Motivated by the quite significant activity exhibited by $R_3\text{PAu}(\text{S}_2\text{CNRR}')$, $R, R' = \text{alkyl/aryl}$ (Sim *et al.*, 2014; Chen *et al.*, 2016), lower congeners, *i.e.* $(\text{Ph}_3\text{P})_2\text{M}(\text{S}_2\text{CNRR}')$, $M = \text{Cu}^{\text{I}}$ and Ag^{I} , were investigated and shown to be also potent in this context (Jamaludin *et al.*, 2016). A prominent lead compound, $\text{Et}_3\text{PAu}(\text{S}_2\text{CNEt}_2)$, was shown to possess broad-range activity against Gram-positive and Gram-negative bacteria and, notably, was also bactericidal against methicillin-resistant *Staphylococcus aureus* (MRSA) (Chen *et al.*, 2016). Given that $\text{Et}_3\text{PAu}(\text{S}_2\text{CNEt}_2)$ exhibited the most exciting potential amongst the phosphane-gold dithiocarbamates, it was thought of interest to extend the chemistry/biological investigations of $(R_3\text{P})_2\text{M}(\text{S}_2\text{CNRR}')$, $M = \text{Cu}^{\text{I}}$ and Ag^{I} , to include trialkyl-phosphane species. It was during these studies that the title compound, (I), was isolated as an incomplete reaction product from the 1:2:1 reaction between CuCl, Et₃P and NH₄[S₂CN(CH₂)₄]. Herein, the crystal and molecular structures of (I) are described along with a detailed analysis of the Hirshfeld surface.





2. Structural commentary

The molecular structure of (I), Fig. 1, represents a neutral, trinuclear Cu^{I} complex comprising three monodentate phosphane ligands, two chlorido anions, one μ_3 - and the other μ_2 -bridging, and a dithiocarbamate ligand. The latter is tetra-coordinating, chelating the Cu_3 atom, and each sulfur atom also bridges another Cu^{I} atom. As highlighted in Fig. 2, the $\text{Cu}_3\text{Cl}_2\text{S}_2$ atoms of the core occupy the corners of a distorted cube with the putative eighth position being occupied by the quaternary-carbon atom of the dithiocarbamate ligand. As listed in Table 1, there are systematic trends in the Cu –donor-atom bond lengths. To a first approximation, the Cu – P bond lengths are about the same. As anticipated for the Cu_1 and Cu_2 atoms, the Cu – Cl bond lengths involving the μ_3 -chlorido ligand are systematically longer than those formed with the μ_2 -chlorido ligand. Despite being chelated by the dithio-

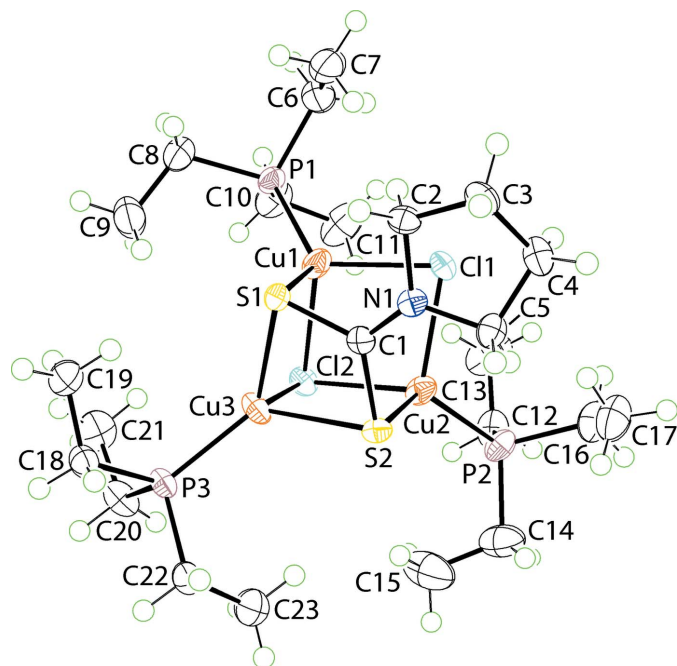


Figure 1

The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

Table 1

Selected geometric parameters (\AA , $^\circ$).

$\text{Cu1}-\text{Cl1}$	2.3474 (5)	$\text{Cu2}-\text{P2}$	2.2018 (6)
$\text{Cu1}-\text{Cl2}$	2.5809 (5)	$\text{Cu3}-\text{Cl2}$	2.3912 (5)
$\text{Cu1}-\text{S1}$	2.3282 (5)	$\text{Cu3}-\text{S1}$	2.4002 (5)
$\text{Cu1}-\text{P1}$	2.1936 (5)	$\text{Cu3}-\text{S2}$	2.4939 (5)
$\text{Cu2}-\text{Cl1}$	2.3640 (5)	$\text{Cu3}-\text{P3}$	2.1841 (5)
$\text{Cu2}-\text{Cl2}$	2.5324 (5)	$\text{S1}-\text{C1}$	1.7367 (19)
$\text{Cu2}-\text{S2}$	2.3556 (5)	$\text{S2}-\text{C1}$	1.7330 (19)
$\text{Cl1}-\text{Cu1}-\text{Cl2}$	96.188 (18)	$\text{Cl2}-\text{Cu2}-\text{S2}$	97.904 (18)
$\text{Cl1}-\text{Cu1}-\text{S1}$	104.585 (19)	$\text{Cl2}-\text{Cu2}-\text{P2}$	112.82 (2)
$\text{Cl1}-\text{Cu1}-\text{P1}$	115.51 (2)	$\text{S2}-\text{Cu2}-\text{P2}$	124.87 (2)
$\text{Cl2}-\text{Cu1}-\text{S1}$	100.954 (18)	$\text{Cl2}-\text{Cu3}-\text{S1}$	104.566 (18)
$\text{Cl2}-\text{Cu1}-\text{P1}$	108.90 (2)	$\text{Cl2}-\text{Cu3}-\text{S2}$	98.030 (18)
$\text{S1}-\text{Cu1}-\text{P1}$	125.81 (2)	$\text{Cl2}-\text{Cu3}-\text{P3}$	118.56 (2)
$\text{Cl1}-\text{Cu2}-\text{Cl2}$	97.080 (18)	$\text{S1}-\text{Cu3}-\text{S2}$	74.935 (17)
$\text{Cl1}-\text{Cu2}-\text{S2}$	106.406 (19)	$\text{S1}-\text{Cu3}-\text{P3}$	127.39 (2)
$\text{Cl1}-\text{Cu2}-\text{P2}$	113.35 (2)	$\text{S2}-\text{Cu3}-\text{P3}$	123.04 (2)

carbamate ligand, the Cu_3 atom forms longer Cu – S bond lengths than do the Cu_1 and Cu_2 atoms, an observation correlated with the presence of two electronegative chloride anions in the donor sets for the latter.

The coordination geometries for the Cu_1 and Cu_2 atoms are based on Cl_2PS donor sets while that of Cu_3 is based on a ClPS_2 donor set, Table 1. While being based on tetrahedra, the coordination geometries exhibit wide ranges of angles subtended at the copper atoms, *i.e.* 30, 28 and 53° , respectively. The wider range of angles about the Cu_3 atom can be traced, in part, to the acute angle subtended by the dithiocarbamate ligand. A measure of the geometry defined by a four-atom donor set is τ_4 (Yang *et al.*, 2007). Based on this index, τ_4 values of 1 and 0 are computed for ideal tetrahedral and square-planar geometries, respectively. The τ_4 values calculated for the Cu_1 – Cu_3 atoms in (I) are 0.84, 0.86 and 0.78, respectively, *i.e.* consistent with distortions from tetrahedral geometries.

Reflecting the near equivalence in the pairs of Cu – S1 and Cu – S2 bonds, the associated C – S bond lengths are equal within experimental error, Table 1. Finally, the pyrrolidine ring is twisted about the C3 – C4 bond.

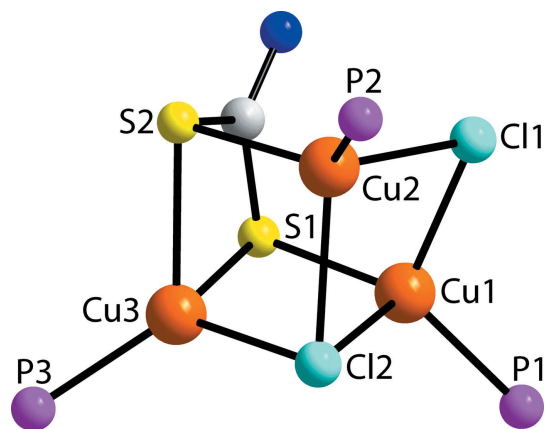


Figure 2

The molecular core in (I) highlighting the 'incomplete cube'.

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

Cg1 is the centroid of the (Cu,S1,S2,C1) chelate ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C20—H20 <i>B</i> ...Cl1 ⁱ	0.99	2.81	3.722 (2)	154
C22—H22 <i>B</i> ...Cl1 ⁱ	0.99	2.80	3.720 (2)	154
C3—H3 <i>B</i> ...Cg1 ⁱⁱ	0.99	2.83	3.705 (2)	148

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

3. Supramolecular features

The key feature of the molecular packing in (I) is the formation of linear supramolecular chains along the *c* axis, Fig. 3*a* and Table 2. The μ₂-chlorido ligand accepts two phosphane-methylene-C—H...Cl type interactions to form a linear chain. Centrosymmetrically related chains are connected *via* pyrrolidine-methylene-C—H...π(chelate) interactions where the chelate ring is defined by the Cu1,S1,S2,C1 atoms. Such C—H...π(chelate) interactions are now well established in dithiocarbamate structural chemistry (Tiekink & Zukerman-Schpector, 2011) and are gaining greater recognition in coordination chemistry (Tiekink, 2017). The supramolecular chains pack in the crystal with no directional interactions between them, Fig. 3*b*.

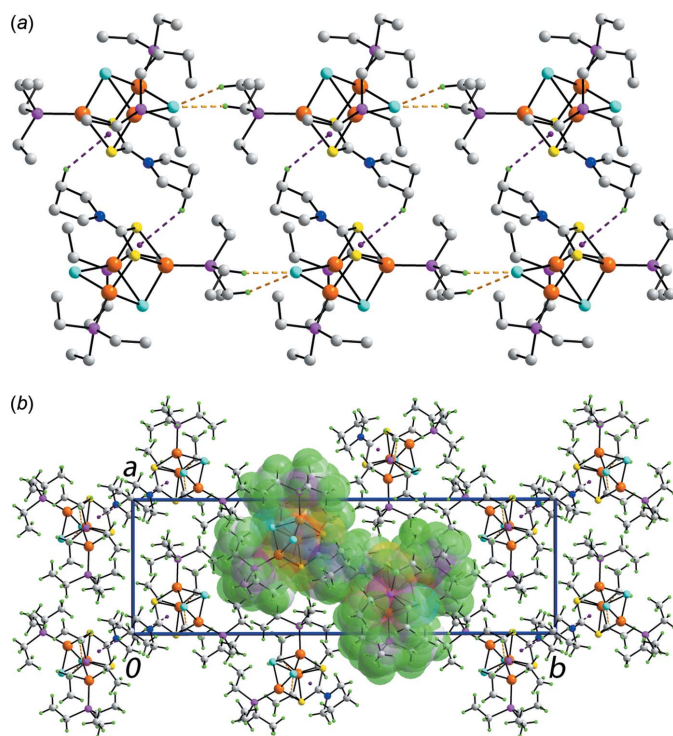


Figure 3
The molecular packing in (I): (a) linear supramolecular chain mediated by methylene-C—H...Cl (orange dashed lines) and methylene-C—H...π(chelate) (blue) interactions aligned along the *c* axis and (b) view of the unit-cell contents in projection down the *c* axis. One chain is highlighted in space-filling mode.

4. Hirshfeld surface analysis

The Hirshfeld surface analysis of (I) was performed in accord with a recent study of a related dithiocarbamate complex (Jotani *et al.*, 2016). The presence of tiny red spots near the Cl1 and methylene-H20*B* and H22*B* atoms on the Hirshfeld surfaces mapped over *d*_{norm} in Fig. 4 is indicative of the double-acceptor (C—H)₂...Cl interaction. In the view of the Hirshfeld surface mapped over the calculated electrostatic potential in Fig. 5, the light-blue and pale-red regions around the electropositive and electronegative atoms result from the polarization of charges about the donors and acceptors, respectively, of the intermolecular interactions. The immediate environments about a reference molecule within the shape-index-mapped Hirshfeld surfaces in Fig. 6*a* and *b* highlight the intermolecular C—H...Cl and C—H...π(chelate) interactions, respectively.

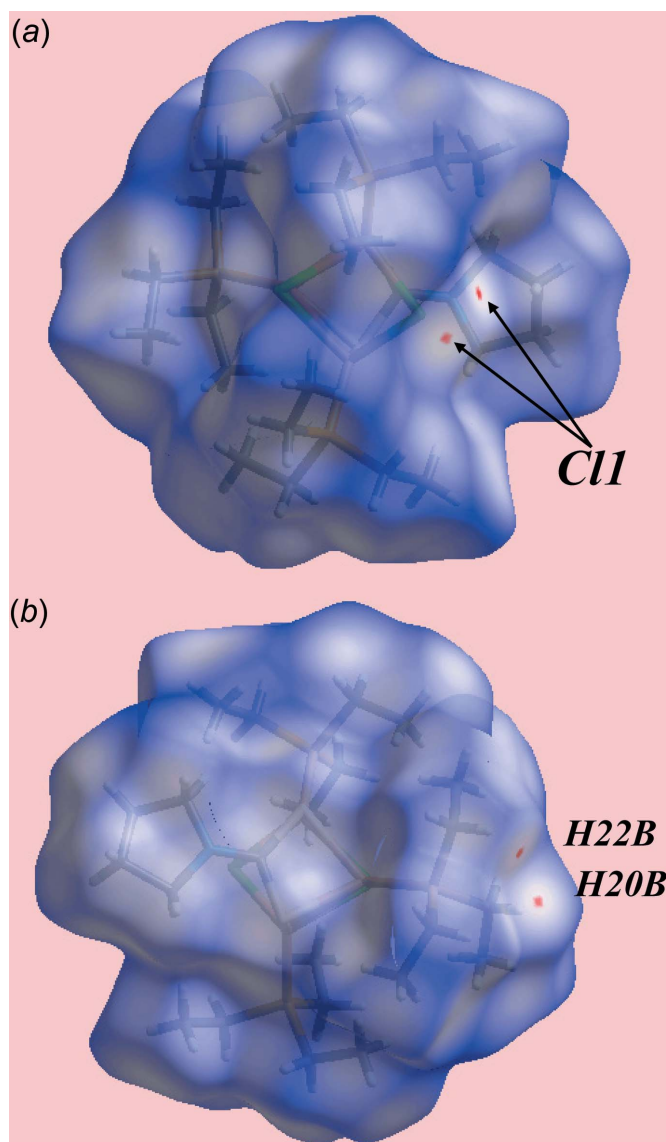


Figure 4
Two views of the Hirshfeld surface for (I) mapped over *d*_{norm} over the range −0.016 to 1.529 au.

Table 3
Percentage contribution of interatomic contacts to the Hirshfeld surface for (I).

Contact	percentage contribution
H··H	86.6
Cl··H/H··Cl	5.8
S··H/H··S	5.7
C··H/H··C	1.1
Cu··H/H··Cu	0.4
N··H/H··N	0.3
C··N/N··C	0.1

The two-dimensional fingerprint plots for (I), *i.e.* the overall, Fig. 7a, and those delineated into H··H, Cl··H/H··Cl and S··H/H··S contacts (McKinnon *et al.*, 2007) in Fig. 7b–d, respectively, provide further information on the intermolecular interactions present in the crystal. It is evident from the fingerprint plot delineated into H··H contacts, Fig. 7b, that the hydrogen atoms of the triethylphosphane and pyrrolidine ligands make the greatest contribution, *i.e.* 86.6%, to the Hirshfeld surface, but at distances greater than the sum of the van der Waals radii. The pair of tips at $d_e + d_i \sim 2.8$ Å in the arrow-like distribution of points in the plot for Cl··H/H··Cl contacts, Fig. 7c, represent the intermolecular C–H··Cl interactions. A pair of short spikes at $d_e + d_i \sim 3.0$ Å in the S··H/H··S delineated plot, Fig. 7d, and the 5.8% contribution to Hirshfeld surfaces along with the small but significant contributions from C··H/H··C and Cu··H/H··Cu contacts, Table 3, to the Hirshfeld surface are all

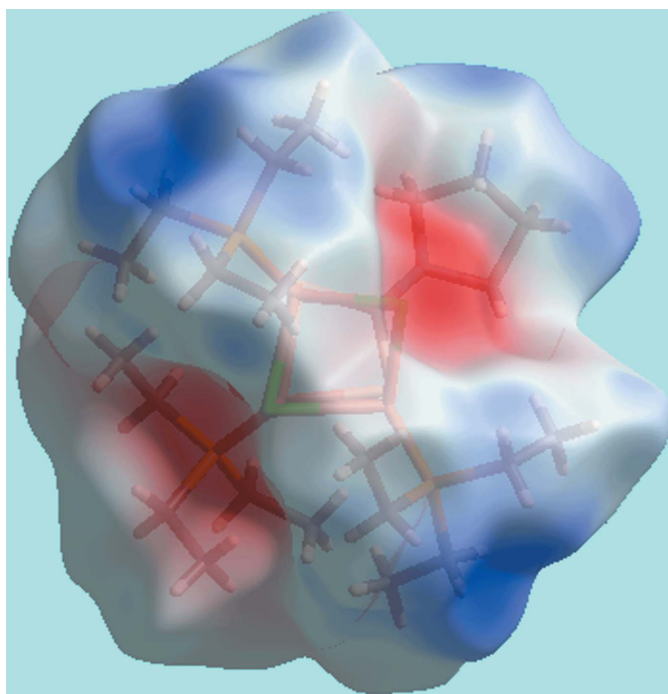


Figure 5
A view of the Hirshfeld surface for (I) mapped over the calculated electrostatic potential in the range -0.071 to 0.030 au. The red and blue regions represent negative and positive electrostatic potentials, respectively.

indicative of the C–H·· π (chelate) interaction, Fig. 3a and Table 2. The small contributions from the other interatomic contacts, namely N··H/H··N and C··N/N··C, have little effect on the packing of the crystal.

5. Database survey

The isolated $\text{Cu}_3(\mu_3\text{-Cl})(\mu_2\text{-Cl})\text{S}_2$ core observed in (I) appears to be rare in the literature, being structurally observed only in one other structure with general formula, $M_3(\mu_3\text{-X})(\mu_2\text{-X})\text{S}_2$, incidentally, a dithiocarbamate complex. Thus, in the Ru^{II} species, $\text{Ru}_3(\text{CO})_5(\text{S}_2\text{CNET}_2)_4\text{Cl}_2$, a discrete $\text{Ru}_3(\mu_3\text{-Cl})(\mu_2\text{-Cl})\text{S}_2$ core is found but where the $\mu_2\text{-S}$ sulfur atoms are derived from four dithiocarbamate ligands and each Ru^{II} atom is coordinated by two additional sulfur donor atoms leading to *trans*- RuCClS_4 octahedral coordination geometries (Raston & White, 1975). While other structures are known with the specified core, the core is embedded within higher nuclearity clusters or in coordination polymers.

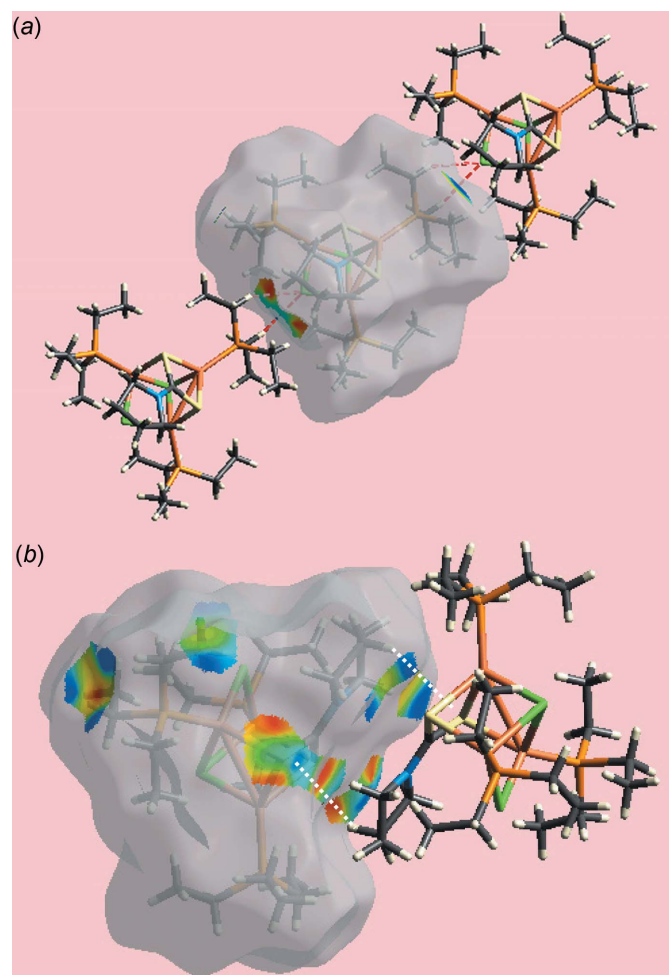
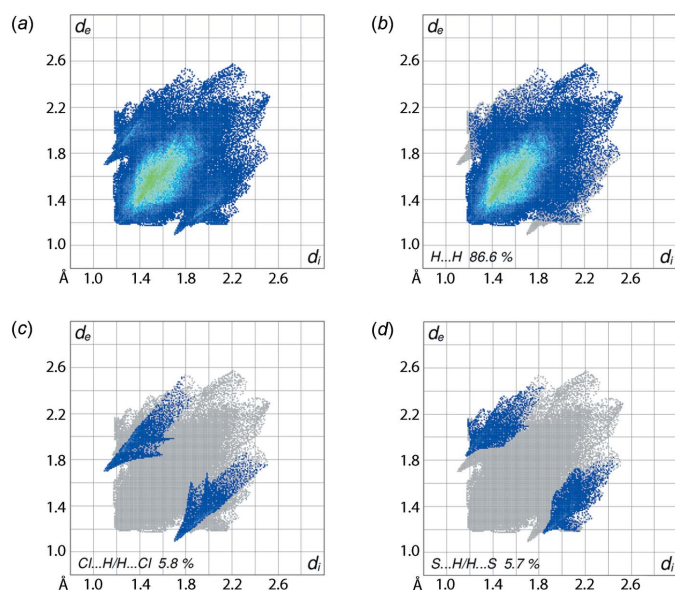


Figure 6
Views of Hirshfeld surface for a reference molecule in (I) mapped over the shape-index property highlighting the: (a) C–H··Cl interactions as red dashed lines and (b) C–H·· π (chelate) interactions as white dashed lines


Figure 7

(a) The full two-dimensional fingerprint plot for (I) and fingerprint plots delineated into (b) H...H, (c) Cl...H/H...Cl and (d) S...H/H...S contacts.

There are twenty crystal structures containing copper with dithiocarbamate and phosphane ligands in the crystallographic literature (Groom *et al.*, 2016). The majority, *i.e.* 12 conform to the tetrahedral CuP_2S_2 motif observed in the biologically active bis(phosphane)copper(I) dithiocarbamate compounds mentioned in the *Chemical Context* (Jamaludin *et al.* 2016; Tan *et al.*, 2016). Similar coordination geometries are found in two binuclear structures with bis(dithiocarbamate) ligands, as exemplified in $(\text{Ph}_3\text{P})_2\text{CuS}_2\text{CN}(\text{CH}_2\text{CH}_2)_2\text{NCS}_2$. $\text{Cu}(\text{PPh}_3)_2$ (Kumar *et al.*, 2009). There are two related complexes but with a 1:1:1 ratio of copper, dithiocarbamate and phosphane, as exemplified by $[\text{Et}_3\text{PCu}(\text{S}_2\text{CNET}_2)]_2$ (Afzaal *et al.*, 2011). One of the remaining structures is neutral and octanuclear with formula $(\text{Ph}_3\text{P})_4\text{Cu}_8(\mu_4\text{-SC}_6\text{H}_4\text{Br-4})_4(\mu_2\text{-SC}_6\text{H}_4\text{Br-4})_2(\text{S}_2\text{CNMe}_2)_2\text{MeO}(\text{CH}_2)_2\text{OMe}$ (Langer *et al.*, 2009). Here, each sulfur atom of the dithiocarbamate ligand bridges two different Cu^{I} atoms. The common feature of the remaining three structures is that they are charged and feature bidentate phosphane ligands. The simplest of these is formulated as $[(\text{dppm})_2\text{Cu}_2(\text{S}_2\text{CNMe}_2)][\text{ClO}_4]_2 \cdot \text{EtOH} \cdot 0.25\text{H}_2\text{O}$ where the dithiocarbamate ligand is bidentate bridging as is the dppm ligand (Huang & Situ, 2003); dppm = $\text{Ph}_2\text{PCH}_2\text{PPh}_2$. In the trinuclear mono-cation $\{(\text{dppm})_3\text{Cu}_3(\mu_3\text{-I})[\text{S}_2\text{CN}(\text{CH}_2\text{Ph})\text{CH}_2(2\text{-thienyl})]\}^+$, the dithiocarbamate ligand bridges two Cu^{I} atoms and simultaneously coordinates a third Cu^{I} atom *via* one of the sulfur atoms only (Rajput *et al.*, 2015). The final structure to be described is related to the former whereby one bis(phosphane) ligand has been replaced by a dithiocarbamate ligand with the ejection of the μ_3 -iodido species, *i.e.* $\{(\text{dppf})_2\text{Cu}_3[\text{S}_2\text{CN}(\text{CH}_2\text{Ph})\text{CH}_2\text{Fc}]_2\}^+\text{PF}_6 \cdot \text{CHCl}_3$ (Kishore *et al.*, 2016); dppf = $\text{Ph}_2\text{P}(\eta^5\text{-C}_5\text{H}_4)\text{Fe}(\eta^5\text{-C}_5\text{H}_4)\text{PPh}_2$ and Fc is $(\eta^5\text{-C}_5\text{H}_4)\text{Fe}(\eta^5\text{-C}_5\text{H}_5)$. In this structure, each dithiocarbamate ligand is tri-coordinate, binding to three different Cu^{I} atoms.

Table 4

Experimental details.

Crystal data	
Chemical formula	$[\text{Cu}_3(\text{C}_5\text{H}_8\text{NS}_2)\text{Cl}_2(\text{C}_6\text{H}_{15}\text{P})_3]$
M_r	762.21
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	10.6489 (2), 31.7578 (4), 10.7212 (2)
β (°)	108.607 (2)
V (Å ³)	3436.24 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	6.14
Crystal size (mm)	0.20 × 0.09 × 0.07
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, AtlasS2
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku Oxford Diffraction, 2015)
$T_{\text{min}}, T_{\text{max}}$	0.684, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34566, 7186, 6699
R_{int}	0.027
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.028, 0.073, 1.04
No. of reflections	7186
No. of parameters	316
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.50, -0.79

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *pubCIF* (Westrip, 2010).

From the foregoing, it is obvious there is considerable structural variability in these systems arising in part from the ability of the dithiocarbamate ligands to adopt quite diverse coordination modes.

6. Synthesis and crystallization

Complex (I) is an unexpected product from the *in situ* reaction of CuCl , Et_3P , and $\text{NH}_4[\text{S}_2\text{CN}(\text{CH}_2)_4]$ in a 1:2:1 ratio. The preparation was as follows: $\text{NH}_4[\text{S}_2\text{CN}(\text{CH}_2)_4]$ (Sigma-Aldrich, 0.5 mmol, 0.082 g) dissolved in isopropanol (5 ml) was added to an isopropanol solution (5 ml) of CuCl (Sigma-Aldrich, 0.5 mmol, 0.05 g) at room temperature. Then, a THF solution of Et_3P (Sigma-Aldrich; 1 ml (= 0.118 g), 1.0 mmol) was added to the reaction mixture followed by stirring for 2 h. The resulting mixture was filtered, diluted with hexane (2 ml) and mixed well. The mixture was left for evaporation at 227 K. A small number of yellow crystals of (I) were obtained after 5 d. Yield: 0.0095 g (4.26%), m.p. 330.8 K. IR (cm⁻¹): 1429(s) $\nu(\text{C}-\text{N})$; 1045(*m*), 993(*m*) $\nu(\text{C}-\text{S})$.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. Carbon-bound H atoms were placed in calculated positions ($\text{C}-\text{H} = 0.98\text{--}0.99$ Å) and were

included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to $1.2\text{--}1.5U_{\text{eq}}(\text{C})$.

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supporting information

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μ_3 -Chlorido- μ_2 -chlorido-(μ_3 -pyrrolidine-1-carbodithioato- κ^4 S:S,S':S')tris[(triethylphosphane- κ P)copper(I)]: crystal structure and Hirshfeld surface analysis

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Computing details

Data collection: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); cell refinement: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); data reduction: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

μ_3 -Chlorido- μ_2 -chlorido-(μ_3 -pyrrolidine-1-carbodithioato- κ^4 S:S,S':S')tris[(triethylphosphane- κ P)copper(I)]

Crystal data

[Cu₃(C₅H₈NS₂)Cl₂(C₆H₁₅P)₃]

$M_r = 762.21$

Monoclinic, $P2_1/n$

$a = 10.6489$ (2) Å

$b = 31.7578$ (4) Å

$c = 10.7212$ (2) Å

$\beta = 108.607$ (2)°

$V = 3436.24$ (11) Å³

$Z = 4$

$F(000) = 1584$

$D_x = 1.473$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 16968 reflections

$\theta = 2.8$ – 76.3 °

$\mu = 6.14$ mm⁻¹

$T = 100$ K

Prism, yellow

$0.20 \times 0.09 \times 0.07$ mm

Data collection

Agilent SuperNova, Dual, Cu at zero, AtlasS2 diffractometer

Radiation source: micro-focus sealed X-ray tube

Mirror monochromator

Detector resolution: 10.4607 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlisPro*; Rigaku Oxford Diffraction, 2015)

$T_{\min} = 0.684$, $T_{\max} = 1.000$

34566 measured reflections

7186 independent reflections

6699 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 76.6$ °, $\theta_{\min} = 2.8$ °

$h = -13 \rightarrow 12$

$k = -39 \rightarrow 29$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.073$

$S = 1.04$

7186 reflections

316 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 3.4591P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.50$ e Å⁻³

$\Delta\rho_{\min} = -0.79$ 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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.15403 (3)	0.60427 (2)	0.46213 (3)	0.02150 (8)
Cu2	0.41213 (3)	0.65484 (2)	0.54323 (3)	0.02075 (8)
Cu3	0.29958 (3)	0.60979 (2)	0.26251 (3)	0.02196 (8)
Cl1	0.29973 (4)	0.62046 (2)	0.67210 (4)	0.01860 (9)
Cl2	0.21102 (4)	0.66892 (2)	0.34453 (4)	0.01933 (9)
S1	0.26010 (4)	0.55091 (2)	0.38531 (4)	0.01620 (9)
S2	0.50822 (4)	0.60146 (2)	0.45081 (4)	0.01641 (9)
P1	-0.05739 (5)	0.60624 (2)	0.44227 (5)	0.01844 (10)
P2	0.51349 (5)	0.71293 (2)	0.63413 (5)	0.02172 (11)
P3	0.29464 (5)	0.61039 (2)	0.05729 (5)	0.01832 (10)
N1	0.46529 (16)	0.53980 (5)	0.60120 (15)	0.0162 (3)
C1	0.41813 (18)	0.56133 (6)	0.49156 (18)	0.0152 (3)
C2	0.38664 (19)	0.50826 (6)	0.64599 (19)	0.0190 (4)
H2A	0.3621	0.4843	0.5840	0.023*
H2B	0.3049	0.5210	0.6546	0.023*
C3	0.4799 (2)	0.49415 (6)	0.78003 (19)	0.0222 (4)
H3A	0.4297	0.4867	0.8403	0.027*
H3B	0.5338	0.4697	0.7709	0.027*
C4	0.5667 (2)	0.53283 (6)	0.82932 (19)	0.0238 (4)
H4A	0.5202	0.5540	0.8665	0.029*
H4B	0.6510	0.5250	0.8972	0.029*
C5	0.59098 (19)	0.54950 (6)	0.70556 (19)	0.0201 (4)
H5A	0.6084	0.5802	0.7119	0.024*
H5B	0.6666	0.5349	0.6896	0.024*
C6	-0.0943 (2)	0.58600 (9)	0.5866 (2)	0.0350 (5)
H6A	-0.0571	0.6055	0.6612	0.042*
H6B	-0.1916	0.5853	0.5674	0.042*
C7	-0.0388 (3)	0.54232 (9)	0.6268 (3)	0.0417 (6)
H7A	-0.0801	0.5224	0.5558	0.063*
H7B	-0.0576	0.5337	0.7068	0.063*
H7C	0.0572	0.5426	0.6437	0.063*
C8	-0.1738 (2)	0.57717 (7)	0.3059 (2)	0.0285 (4)
H8A	-0.1613	0.5466	0.3233	0.034*
H8B	-0.2656	0.5844	0.3014	0.034*
C9	-0.1549 (3)	0.58705 (9)	0.1739 (2)	0.0379 (6)
H9A	-0.1690	0.6172	0.1553	0.057*
H9B	-0.2189	0.5709	0.1043	0.057*
H9C	-0.0647	0.5794	0.1772	0.057*
C10	-0.1319 (2)	0.65879 (8)	0.4228 (3)	0.0332 (5)

H10A	-0.1436	0.6691	0.3326	0.040*
H10B	-0.2207	0.6569	0.4335	0.040*
C11	-0.0480 (3)	0.69041 (8)	0.5220 (3)	0.0432 (6)
H11A	-0.0424	0.6817	0.6112	0.065*
H11B	-0.0890	0.7183	0.5040	0.065*
H11C	0.0412	0.6915	0.5144	0.065*
C12	0.4059 (2)	0.75778 (7)	0.6313 (2)	0.0287 (5)
H12A	0.4587	0.7807	0.6861	0.034*
H12B	0.3690	0.7683	0.5400	0.034*
C13	0.2925 (3)	0.74600 (9)	0.6827 (3)	0.0435 (6)
H13A	0.2441	0.7219	0.6328	0.065*
H13B	0.2322	0.7700	0.6723	0.065*
H13C	0.3284	0.7385	0.7761	0.065*
C14	0.6344 (3)	0.73513 (8)	0.5657 (3)	0.0387 (6)
H14A	0.6573	0.7640	0.5999	0.046*
H14B	0.7163	0.7180	0.5937	0.046*
C15	0.5811 (4)	0.73634 (9)	0.4171 (3)	0.0517 (8)
H15A	0.5621	0.7076	0.3830	0.078*
H15B	0.6471	0.7491	0.3828	0.078*
H15C	0.4995	0.7531	0.3893	0.078*
C16	0.6077 (2)	0.70895 (7)	0.8114 (2)	0.0322 (5)
H16A	0.6675	0.7335	0.8377	0.039*
H16B	0.5451	0.7098	0.8626	0.039*
C17	0.6886 (3)	0.66909 (9)	0.8443 (3)	0.0393 (6)
H17A	0.6292	0.6447	0.8289	0.059*
H17B	0.7439	0.6697	0.9369	0.059*
H17C	0.7454	0.6669	0.7884	0.059*
C18	0.2471 (2)	0.56150 (6)	-0.03875 (19)	0.0223 (4)
H18A	0.2167	0.5687	-0.1335	0.027*
H18B	0.3265	0.5434	-0.0219	0.027*
C19	0.1383 (2)	0.53638 (7)	-0.0080 (2)	0.0291 (5)
H19A	0.1670	0.5292	0.0858	0.044*
H19B	0.1209	0.5105	-0.0604	0.044*
H19C	0.0573	0.5533	-0.0297	0.044*
C20	0.1873 (2)	0.65065 (7)	-0.0452 (2)	0.0262 (4)
H20A	0.2228	0.6788	-0.0128	0.031*
H20B	0.1890	0.6478	-0.1366	0.031*
C21	0.0443 (2)	0.64775 (8)	-0.0457 (2)	0.0336 (5)
H21A	0.0058	0.6210	-0.0855	0.050*
H21B	-0.0069	0.6712	-0.0969	0.050*
H21C	0.0422	0.6492	0.0448	0.050*
C22	0.4553 (2)	0.62219 (7)	0.0359 (2)	0.0237 (4)
H22A	0.5156	0.5980	0.0675	0.028*
H22B	0.4427	0.6259	-0.0590	0.028*
C23	0.5198 (3)	0.66167 (8)	0.1099 (2)	0.0358 (5)
H23A	0.4631	0.6861	0.0754	0.054*
H23B	0.6064	0.6660	0.0981	0.054*
H23C	0.5312	0.6583	0.2038	0.054*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01310 (14)	0.02656 (16)	0.02473 (15)	-0.00123 (11)	0.00588 (11)	-0.00501 (12)
Cu2	0.02180 (15)	0.01514 (14)	0.02611 (15)	-0.00383 (11)	0.00876 (12)	-0.00443 (11)
Cu3	0.03038 (17)	0.02277 (15)	0.01416 (14)	0.00065 (12)	0.00914 (12)	0.00068 (11)
Cl1	0.0220 (2)	0.0212 (2)	0.01358 (18)	0.00073 (16)	0.00701 (16)	-0.00123 (15)
Cl2	0.0218 (2)	0.0185 (2)	0.0179 (2)	0.00308 (16)	0.00661 (17)	0.00183 (15)
S1	0.0173 (2)	0.0152 (2)	0.0159 (2)	-0.00239 (15)	0.00490 (16)	-0.00200 (15)
S2	0.0158 (2)	0.0155 (2)	0.0199 (2)	-0.00078 (15)	0.00855 (17)	-0.00004 (16)
P1	0.0128 (2)	0.0219 (2)	0.0203 (2)	-0.00112 (17)	0.00482 (18)	-0.00132 (18)
P2	0.0190 (2)	0.0146 (2)	0.0294 (3)	-0.00147 (17)	0.0047 (2)	-0.00271 (19)
P3	0.0240 (2)	0.0181 (2)	0.0136 (2)	0.00122 (18)	0.00702 (18)	-0.00037 (17)
N1	0.0171 (7)	0.0130 (7)	0.0189 (7)	0.0005 (6)	0.0064 (6)	-0.0003 (6)
C1	0.0172 (8)	0.0131 (8)	0.0169 (8)	0.0018 (6)	0.0078 (7)	-0.0028 (6)
C2	0.0225 (9)	0.0150 (9)	0.0210 (9)	0.0001 (7)	0.0088 (8)	0.0029 (7)
C3	0.0296 (11)	0.0186 (9)	0.0196 (9)	0.0032 (8)	0.0096 (8)	0.0026 (7)
C4	0.0299 (11)	0.0213 (10)	0.0177 (9)	0.0030 (8)	0.0038 (8)	-0.0001 (7)
C5	0.0190 (9)	0.0173 (9)	0.0212 (9)	0.0013 (7)	0.0024 (7)	0.0000 (7)
C6	0.0254 (11)	0.0531 (15)	0.0265 (11)	-0.0062 (10)	0.0082 (9)	0.0025 (10)
C7	0.0346 (13)	0.0498 (16)	0.0327 (12)	-0.0154 (11)	-0.0005 (10)	0.0135 (11)
C8	0.0230 (10)	0.0317 (11)	0.0286 (11)	-0.0046 (9)	0.0050 (8)	-0.0029 (9)
C9	0.0364 (13)	0.0504 (15)	0.0243 (11)	-0.0012 (11)	0.0062 (10)	-0.0042 (10)
C10	0.0245 (11)	0.0307 (12)	0.0426 (13)	0.0035 (9)	0.0083 (10)	-0.0036 (10)
C11	0.0314 (13)	0.0334 (13)	0.0651 (18)	-0.0017 (10)	0.0159 (12)	-0.0186 (12)
C12	0.0337 (12)	0.0184 (10)	0.0300 (11)	0.0038 (8)	0.0045 (9)	-0.0029 (8)
C13	0.0337 (13)	0.0317 (13)	0.0680 (18)	0.0024 (10)	0.0204 (13)	-0.0126 (12)
C14	0.0443 (14)	0.0300 (12)	0.0513 (15)	-0.0103 (10)	0.0286 (13)	-0.0079 (11)
C15	0.085 (2)	0.0332 (14)	0.0538 (17)	-0.0146 (14)	0.0455 (17)	-0.0111 (12)
C16	0.0313 (12)	0.0290 (11)	0.0310 (11)	-0.0019 (9)	0.0027 (9)	-0.0041 (9)
C17	0.0324 (13)	0.0386 (14)	0.0374 (13)	-0.0003 (10)	-0.0021 (10)	0.0007 (11)
C18	0.0281 (10)	0.0209 (9)	0.0181 (9)	-0.0013 (8)	0.0076 (8)	-0.0014 (7)
C19	0.0319 (12)	0.0264 (11)	0.0281 (11)	-0.0069 (9)	0.0084 (9)	-0.0022 (8)
C20	0.0341 (11)	0.0236 (10)	0.0232 (10)	0.0101 (8)	0.0123 (9)	0.0034 (8)
C21	0.0300 (12)	0.0345 (12)	0.0349 (12)	0.0096 (9)	0.0082 (10)	0.0020 (10)
C22	0.0269 (10)	0.0260 (10)	0.0185 (9)	-0.0022 (8)	0.0074 (8)	-0.0019 (8)
C23	0.0417 (14)	0.0367 (13)	0.0304 (12)	-0.0135 (11)	0.0132 (10)	-0.0083 (10)

Geometric parameters (\AA , $^\circ$)

Cu1—Cl1	2.3474 (5)	C8—H8B	0.9900
Cu1—Cl2	2.5809 (5)	C9—H9A	0.9800
Cu1—S1	2.3282 (5)	C9—H9B	0.9800
Cu1—P1	2.1936 (5)	C9—H9C	0.9800
Cu2—Cl1	2.3640 (5)	C10—C11	1.527 (3)
Cu2—Cl2	2.5324 (5)	C10—H10A	0.9900
Cu2—S2	2.3556 (5)	C10—H10B	0.9900
Cu2—P2	2.2018 (6)	C11—H11A	0.9800

Cu3—C12	2.3912 (5)	C11—H11B	0.9800
Cu3—S1	2.4002 (5)	C11—H11C	0.9800
Cu3—S2	2.4939 (5)	C12—C13	1.526 (4)
Cu3—P3	2.1841 (5)	C12—H12A	0.9900
Cu1—Cu3	3.0216 (4)	C12—H12B	0.9900
S1—C1	1.7367 (19)	C13—H13A	0.9800
S2—C1	1.7330 (19)	C13—H13B	0.9800
P1—C10	1.831 (2)	C13—H13C	0.9800
P1—C8	1.836 (2)	C14—C15	1.511 (4)
P1—C6	1.830 (2)	C14—H14A	0.9900
P2—C14	1.816 (2)	C14—H14B	0.9900
P2—C12	1.822 (2)	C15—H15A	0.9800
P2—C16	1.849 (2)	C15—H15B	0.9800
P3—C20	1.830 (2)	C15—H15C	0.9800
P3—C22	1.836 (2)	C16—C17	1.508 (3)
P3—C18	1.842 (2)	C16—H16A	0.9900
N1—C1	1.313 (2)	C16—H16B	0.9900
N1—C5	1.477 (2)	C17—H17A	0.9800
N1—C2	1.480 (2)	C17—H17B	0.9800
C2—C3	1.530 (3)	C17—H17C	0.9800
C2—H2A	0.9900	C18—C19	1.526 (3)
C2—H2B	0.9900	C18—H18A	0.9900
C3—C4	1.527 (3)	C18—H18B	0.9900
C3—H3A	0.9900	C19—H19A	0.9800
C3—H3B	0.9900	C19—H19B	0.9800
C4—C5	1.526 (3)	C19—H19C	0.9800
C4—H4A	0.9900	C20—C21	1.523 (3)
C4—H4B	0.9900	C20—H20A	0.9900
C5—H5A	0.9900	C20—H20B	0.9900
C5—H5B	0.9900	C21—H21A	0.9800
C6—C7	1.515 (4)	C21—H21B	0.9800
C6—H6A	0.9900	C21—H21C	0.9800
C6—H6B	0.9900	C22—C23	1.525 (3)
C7—H7A	0.9800	C22—H22A	0.9900
C7—H7B	0.9800	C22—H22B	0.9900
C7—H7C	0.9800	C23—H23A	0.9800
C8—C9	1.524 (3)	C23—H23B	0.9800
C8—H8A	0.9900	C23—H23C	0.9800
C11—Cu1—C12	96.188 (18)	C9—C8—P1	112.35 (16)
C11—Cu1—S1	104.585 (19)	C9—C8—H8A	109.1
C11—Cu1—P1	115.51 (2)	P1—C8—H8A	109.1
C12—Cu1—S1	100.954 (18)	C9—C8—H8B	109.1
C12—Cu1—P1	108.90 (2)	P1—C8—H8B	109.1
S1—Cu1—P1	125.81 (2)	H8A—C8—H8B	107.9
C11—Cu2—C12	97.080 (18)	C8—C9—H9A	109.5
C11—Cu2—S2	106.406 (19)	C8—C9—H9B	109.5
C11—Cu2—P2	113.35 (2)	H9A—C9—H9B	109.5

C12—Cu2—S2	97.904 (18)	C8—C9—H9C	109.5
C12—Cu2—P2	112.82 (2)	H9A—C9—H9C	109.5
S2—Cu2—P2	124.87 (2)	H9B—C9—H9C	109.5
C12—Cu3—S1	104.566 (18)	C11—C10—P1	112.60 (17)
C12—Cu3—S2	98.030 (18)	C11—C10—H10A	109.1
C12—Cu3—P3	118.56 (2)	P1—C10—H10A	109.1
S1—Cu3—S2	74.935 (17)	C11—C10—H10B	109.1
S1—Cu3—P3	127.39 (2)	P1—C10—H10B	109.1
S2—Cu3—P3	123.04 (2)	H10A—C10—H10B	107.8
P1—Cu1—Cu3	132.231 (19)	C10—C11—H11A	109.5
S1—Cu1—Cu3	51.338 (13)	C10—C11—H11B	109.5
C11—Cu1—Cu3	109.575 (16)	H11A—C11—H11B	109.5
C12—Cu1—Cu3	49.769 (12)	C10—C11—H11C	109.5
P3—Cu3—Cu1	149.44 (2)	H11A—C11—H11C	109.5
C12—Cu3—Cu1	55.492 (13)	H11B—C11—H11C	109.5
S1—Cu3—Cu1	49.237 (13)	C13—C12—P2	111.61 (16)
S2—Cu3—Cu1	86.926 (14)	C13—C12—H12A	109.3
Cu1—C11—Cu2	81.004 (17)	P2—C12—H12A	109.3
Cu3—C12—Cu2	81.010 (16)	C13—C12—H12B	109.3
Cu3—C12—Cu1	74.739 (16)	P2—C12—H12B	109.3
Cu2—C12—Cu1	73.508 (15)	H12A—C12—H12B	108.0
C1—S1—Cu1	96.15 (6)	C12—C13—H13A	109.5
C1—S1—Cu3	84.76 (6)	C12—C13—H13B	109.5
Cu1—S1—Cu3	79.425 (17)	H13A—C13—H13B	109.5
C1—S2—Cu2	94.21 (6)	C12—C13—H13C	109.5
C1—S2—Cu3	81.97 (6)	H13A—C13—H13C	109.5
Cu2—S2—Cu3	82.517 (17)	H13B—C13—H13C	109.5
C10—P1—C8	102.12 (11)	C15—C14—P2	111.1 (2)
C10—P1—C6	102.40 (12)	C15—C14—H14A	109.4
C8—P1—C6	102.94 (11)	P2—C14—H14A	109.4
C10—P1—Cu1	115.53 (8)	C15—C14—H14B	109.4
C8—P1—Cu1	118.31 (8)	P2—C14—H14B	109.4
C6—P1—Cu1	113.48 (8)	H14A—C14—H14B	108.0
C14—P2—C12	102.29 (12)	C14—C15—H15A	109.5
C14—P2—C16	102.70 (13)	C14—C15—H15B	109.5
C12—P2—C16	101.70 (11)	H15A—C15—H15B	109.5
C14—P2—Cu2	117.20 (8)	C14—C15—H15C	109.5
C12—P2—Cu2	115.53 (8)	H15A—C15—H15C	109.5
C16—P2—Cu2	115.24 (8)	H15B—C15—H15C	109.5
C20—P3—C22	102.17 (10)	C17—C16—P2	112.33 (17)
C20—P3—C18	104.21 (10)	C17—C16—H16A	109.1
C22—P3—C18	101.71 (10)	P2—C16—H16A	109.1
C20—P3—Cu3	114.89 (7)	C17—C16—H16B	109.1
C22—P3—Cu3	113.81 (7)	P2—C16—H16B	109.1
C18—P3—Cu3	118.01 (7)	H16A—C16—H16B	107.9
C1—N1—C5	124.37 (16)	C16—C17—H17A	109.5
C1—N1—C2	123.24 (16)	C16—C17—H17B	109.5
C5—N1—C2	111.41 (15)	H17A—C17—H17B	109.5

N1—C1—S2	121.62 (14)	C16—C17—H17C	109.5
N1—C1—S1	120.11 (14)	H17A—C17—H17C	109.5
S2—C1—S1	118.25 (11)	H17B—C17—H17C	109.5
N1—C2—C3	103.77 (16)	C19—C18—P3	114.33 (14)
N1—C2—H2A	111.0	C19—C18—H18A	108.7
C3—C2—H2A	111.0	P3—C18—H18A	108.7
N1—C2—H2B	111.0	C19—C18—H18B	108.7
C3—C2—H2B	111.0	P3—C18—H18B	108.7
H2A—C2—H2B	109.0	H18A—C18—H18B	107.6
C4—C3—C2	103.25 (15)	C18—C19—H19A	109.5
C4—C3—H3A	111.1	C18—C19—H19B	109.5
C2—C3—H3A	111.1	H19A—C19—H19B	109.5
C4—C3—H3B	111.1	C18—C19—H19C	109.5
C2—C3—H3B	111.1	H19A—C19—H19C	109.5
H3A—C3—H3B	109.1	H19B—C19—H19C	109.5
C5—C4—C3	103.30 (16)	C21—C20—P3	113.07 (16)
C5—C4—H4A	111.1	C21—C20—H20A	109.0
C3—C4—H4A	111.1	P3—C20—H20A	109.0
C5—C4—H4B	111.1	C21—C20—H20B	109.0
C3—C4—H4B	111.1	P3—C20—H20B	109.0
H4A—C4—H4B	109.1	H20A—C20—H20B	107.8
N1—C5—C4	102.84 (16)	C20—C21—H21A	109.5
N1—C5—H5A	111.2	C20—C21—H21B	109.5
C4—C5—H5A	111.2	H21A—C21—H21B	109.5
N1—C5—H5B	111.2	C20—C21—H21C	109.5
C4—C5—H5B	111.2	H21A—C21—H21C	109.5
H5A—C5—H5B	109.1	H21B—C21—H21C	109.5
C7—C6—P1	113.13 (18)	C23—C22—P3	112.66 (16)
C7—C6—H6A	109.0	C23—C22—H22A	109.1
P1—C6—H6A	109.0	P3—C22—H22A	109.1
C7—C6—H6B	109.0	C23—C22—H22B	109.1
P1—C6—H6B	109.0	P3—C22—H22B	109.1
H6A—C6—H6B	107.8	H22A—C22—H22B	107.8
C6—C7—H7A	109.5	C22—C23—H23A	109.5
C6—C7—H7B	109.5	C22—C23—H23B	109.5
H7A—C7—H7B	109.5	H23A—C23—H23B	109.5
C6—C7—H7C	109.5	C22—C23—H23C	109.5
H7A—C7—H7C	109.5	H23A—C23—H23C	109.5
H7B—C7—H7C	109.5	H23B—C23—H23C	109.5
C5—N1—C1—S2	6.0 (2)	C6—P1—C8—C9	-176.38 (18)
C2—N1—C1—S2	173.70 (13)	Cu1—P1—C8—C9	-50.4 (2)
C5—N1—C1—S1	-172.23 (14)	C8—P1—C10—C11	-176.76 (19)
C2—N1—C1—S1	-4.5 (2)	C6—P1—C10—C11	76.9 (2)
Cu2—S2—C1—N1	-93.58 (15)	Cu1—P1—C10—C11	-47.0 (2)
Cu3—S2—C1—N1	-175.40 (15)	C14—P2—C12—C13	178.71 (19)
Cu2—S2—C1—S1	84.66 (10)	C16—P2—C12—C13	-75.3 (2)
Cu3—S2—C1—S1	2.84 (9)	Cu2—P2—C12—C13	50.2 (2)

Cu1—S1—C1—N1	96.59 (14)	C12—P2—C14—C15	-81.4 (2)
Cu3—S1—C1—N1	175.33 (15)	C16—P2—C14—C15	173.45 (19)
Cu1—S1—C1—S2	-81.67 (10)	Cu2—P2—C14—C15	46.1 (2)
Cu3—S1—C1—S2	-2.93 (9)	C14—P2—C16—C17	-84.3 (2)
C1—N1—C2—C3	-176.54 (16)	C12—P2—C16—C17	170.03 (19)
C5—N1—C2—C3	-7.4 (2)	Cu2—P2—C16—C17	44.3 (2)
N1—C2—C3—C4	28.69 (19)	C20—P3—C18—C19	-91.44 (17)
C2—C3—C4—C5	-39.4 (2)	C22—P3—C18—C19	162.62 (16)
C1—N1—C5—C4	152.09 (17)	Cu3—P3—C18—C19	37.36 (18)
C2—N1—C5—C4	-16.9 (2)	C22—P3—C20—C21	179.63 (16)
C3—C4—C5—N1	34.37 (19)	C18—P3—C20—C21	74.03 (18)
C10—P1—C6—C7	-178.43 (18)	Cu3—P3—C20—C21	-56.63 (18)
C8—P1—C6—C7	75.85 (19)	C20—P3—C22—C23	73.77 (18)
Cu1—P1—C6—C7	-53.22 (19)	C18—P3—C22—C23	-178.70 (16)
C10—P1—C8—C9	77.7 (2)	Cu3—P3—C22—C23	-50.70 (18)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the (Cu,S1,S2,C1) chelate ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C20—H20 <i>B</i> ...C11 ⁱ	0.99	2.81	3.722 (2)	154
C22—H22 <i>B</i> ...C11 ⁱ	0.99	2.80	3.720 (2)	154
C3—H3 <i>B</i> ...Cg1 ⁱⁱ	0.99	2.83	3.705 (2)	148

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