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Copper(I) iodide ribbons coordinated with thiourea derivatives

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Two products of the reactions of CuI with 1-benzoyl-3-(4-bromophenyl)thiourea and with 1-benzoyl-3-(2-iodophenyl)thiourea have been obtained and characterized, namely poly[[[1-benzoyl-3-(4-bromophenyl)thiourea-κS]-μ_3-iodido-copper(I)] acetone hemisolvate], $\{[CuI(C_{14}H_{11}BrN_2OS)]\cdot 0.5C_3H_6O\}_n$, and poly-[$\mu_4$-iodido-$\mu_3$-iodido-[*N*-(benzo[*d*]thiazol-2-yl)benzamide-κN]dicopper(I)], $[Cu_2I_2(C_{14}H_{10}N_2OS)]_n$. Their structures, determined by single-crystal X-ray diffraction analysis, exhibit different stoichiometries and molecular organizations; however, both compounds are polymeric and possess close Cu···Cu contacts. The first product contains a $(CuI)_n$ double chain supported by the thiourea derivative coordinated *via* the S atom. In the second case, the ligand undergoes dehalogenation and cyclization to form *N*-(benzo[*d*]thiazol-2-yl)benzamide that serves as the *N*-donor ligand which is connected to both sides of a $(CuI)_n$ quadruple chain. In both hybrid inorganic chains, I atoms bridge three or four Cu atoms. The coordination centres adopt more or less distorted tetrahedral geometries. The structures of the $(CuI)_n$ kernels of the ribbons are similar to fragments of the layers in high-pressure phase V copper(I) iodide. Only weak S···O, C—H···O, C—H···I and π–π interactions hold the ribbons together, allowing the formation of crystals.

1. Introduction

During our systematic research, we reacted d^{10} metal halides with 3-substituted 1-benzoylthioureas (Okuniewski *et al.*, 2015; Rosiak *et al.*, 2018). For many years, scientists have paid much attention to 3-substituted 1-acylthioureas due to their variable topological aspects, binding modes and susceptibility to side reactions, *e.g.* cyclization (Saeed *et al.*, 2013, 2016). As soft Lewis bases, they readily form complexes with soft Lewis acids, such as copper, gold and mercury ions (Mirzaei *et al.*, 2013), where they serve as *S*-donor ligands.

As part of our research, we attempted to obtain hybrid inorganic–organic frameworks that fascinate not only with their structural diversity but, more importantly, with the wide range of possibilities of designing new materials (Loukopoulos & Kostakis, 2018). The design of crystals is based mainly on the prediction of the spatial distribution of coordination polyhedra, linkers and hydrogen bonds. Currently, increasing attention is being paid to weak interactions, such as halogen, chalcogen, π–π and metallophilic interactions (Jeannin *et al.*, 2018; Zhang & Wang, 2018; Ateş *et al.*, 2018; Romanova *et al.*, 2016; Yao *et al.*, 2017).

The development of coordination compounds based on linearly arranged metal atoms that potentially serve as conducting wires in molecular microelectronics has made tremendous progress in recent years (Berry, 2005; Georgiev *et al.*, 2013). $Au^I\cdots Au^I$ aurophilic interactions, which generally originate from relativistic and correlation effects, are com-

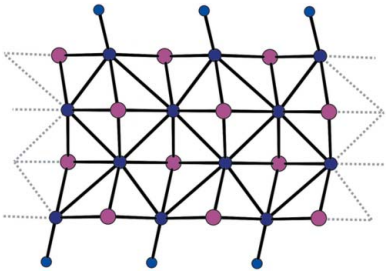

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Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[CuBrI(C_{14}H_{11}N_2OS)]\cdot 0.5C_3H_6O$	$[Cu_2I_2(C_{14}H_{10}N_2OS)]$
M_r	554.70	635.18
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1$
Temperature (K)	120	120
a, b, c (Å)	4.0594 (3), 10.8684 (8), 20.7336 (15)	12.6880 (12), 4.1152 (4), 15.8952 (15)
α, β, γ (°)	102.079 (6), 94.047 (6), 94.299 (6)	90, 100.258 (8), 90
V (Å^3)	888.48 (11)	816.68 (14)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	5.34	6.51
Crystal size (mm)	0.44 × 0.02 × 0.02	0.57 × 0.09 × 0.06
Data collection		
Diffractometer	Stoe IPDS 2T	Stoe IPDS 2T
Absorption correction	Integration [*X-RED32* (Stoe & Cie, 2009), by Gaussian integration, analogous to Coppens (1970)]	Integration [*X-RED32* (Stoe & Cie, 2009), by Gaussian integration, analogous to Coppens (1970)]
T_{min}, T_{max}	0.358, 0.905	0.175, 0.688
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7687, 3446, 3069	7646, 3163, 3139
R_{int}	0.048	0.039
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.175, 1.07	0.044, 0.121, 1.06
No. of reflections	3446	3163
No. of parameters	257	199
No. of restraints	40	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.89, −2.96	1.31, −2.03
Absolute structure	–	Flack x determined using 1322 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	–	0.11 (6)

Computer programs: *X-AREA* (Stoe & Cie, 2009), *X-RED32* (Stoe & Cie, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

parable in strength to hydrogen bonds (Pyykkö, 2004; Paliwoda *et al.*, 2014). Because of the decrease of relativistic effects with decreasing nuclear charge, $Ag^I\cdots Ag^I$ argentophilic bonding is less pronounced and $Cu^I\cdots Cu^I$ cuprophilic interactions are considered to be weak or not significant at all (Dinda & Samuelson, 2012). Except for rare examples of

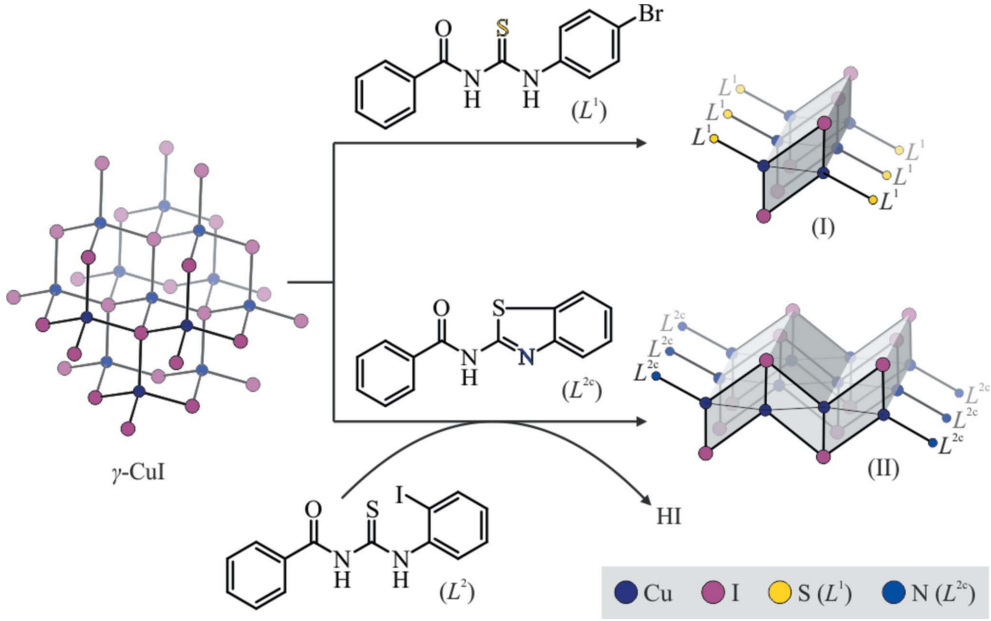

Figure 1
The preparation scheme of complexes (I) and (II).

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unsupported $Cu^{I}\cdots Cu^{I}$ contacts (Oakley *et al.*, 2004; Zheng *et al.*, 2005; Chiarella *et al.*, 2010), multinuclear Cu^{I} complexes exhibiting cuprophilic interactions usually require a suitable ligand framework to incorporate the cuprous ions in close proximity to each other (Stollenz *et al.*, 2016).

In this article, we describe two novel hybrid inorganic chains (Cheetham *et al.*, 2006) in the form of $(CuI)_n$ double, (I), and quadruple ribbons, (II), coordinated with thiourea-related ligands. In both, close Cu···Cu contacts are found.

2. Experimental

Melting points were measured on an SMP30 (Stuart, Stone, United Kingdom) and were uncorrected. The solid-state IR spectra were measured using a Nicolet iS50 FT–IR spectrometer equipped with a Specac Quest single-reflection diamond attenuated total reflectance (ATR) accessory controlled by Omnic computer software in the range 4000–400 cm^{-1}. NMR spectral measurements were performed on a Bruker Avance III HD 400 MHz spectrometer (USA) with a TXI $^{1}H/^{13}C/^{31}P$ probe.

2.1. Synthesis and crystallization

1-Benzoyl-3-(4-bromophenyl)thiourea (L^1) and 1-benzoyl-3-(2-iodophenyl)thiourea (L^2) were prepared according to standard procedures described in our previous work (Okuniewski *et al.*, 2017).

For the synthesis of complexes (I) and (II) (see Fig. 1), copper(I) iodide (4 mmol) and the thiourea derivative (1 mmol; L^1 or L^2) were added to acetone (50 ml). The mixture was stirred and refluxed for 30 min and then allowed to cool. After the mixture had been filtered, the filtrate was left to evaporate slowly at room temperature. In both cases, single crystals suitable for X-ray diffraction analysis were isolated.

2.2. Analytical data

For (I), 0.761 g of CuI and 0.335 g of L^1 were used. After a few days, colourless needles were isolated [m.p. 419 (1) K]. IR (ATR, cm^{-1}): $\nu_{C=O}$ 1672, ν_{N-H} 3401 and 3258. ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.67 (*s*, 1H), 9.39 (*s*, 1H), 8.41–6.99 (*m*, 9H).

For (II), 0.761 g of CuI and 0.382 g of L^2 were used. After a few days, brownish needles were isolated [m.p. 565 (1) K]. IR (ATR, cm^{-1}): $\nu_{C=O}$ 1678, ν_{N-H} absent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51–7.46 (*m*, 9H), 14.02 (*s*, 1H).

2.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed at calculated positions (C—H = 0.95–0.98 Å and N—H = 0.88 Å) and treated as riding on their parent atoms, with $U_{iso}(H)$ values set at 1.2–1.5U_{eq}(C) or 1.2U_{eq}(N).

3. Results and discussion

Compound (I) crystallizes in the triclinic space group $P\overline{1}$. The asymmetric unit contains one molecule of acetone and one molecule of L^1 connected *via* the S atom to a CuI moiety. The thiourea ligand adopts an *S*-type conformation (Woldu & Dillen, 2008), with intramolecular N2—H2···O1 hydrogen bonds forming an *S*(6) motif (Etter, 1990), which is common among 3-monosubstituted 1-acylthioureas (Okuniewski *et al.*, 2012). The resulting six-membered pseudo-rings are quasi-aromatic (Karabiyik *et al.*, 2012) and interact with each other, with the distance being equal to the crystallographic *a*-axis length [4.0594 (3) Å], which is very close to the values reported previously by us for other benzoylthiourea ligands (4.00–4.06; Okuniewski *et al.*, 2017). The structure is also stabilized by classical phenyl–phenyl and bromophenyl–bromophenyl π-stacking interactions, where the distance between the centroids of the rings is also equal to the *a*-axis length; the slippages are 2.20 (2) and 2.27 (2) Å, respectively. Besides N2—H2···O1, weaker N1—H1···I1^{i} hydrogen bonds can also be found in the structure (for hydrogen-bond parameters, see Table 2).

In a difference Fourier map, we observed high residual electron density (maximum peak 6.6 e $Å^{-3}$). The peaks were arranged regularly suggesting the possibility of the presence of disorder over three positions. The disorder was modelled for heavy atoms only (Cu, I, Br and S), as the contribution of the

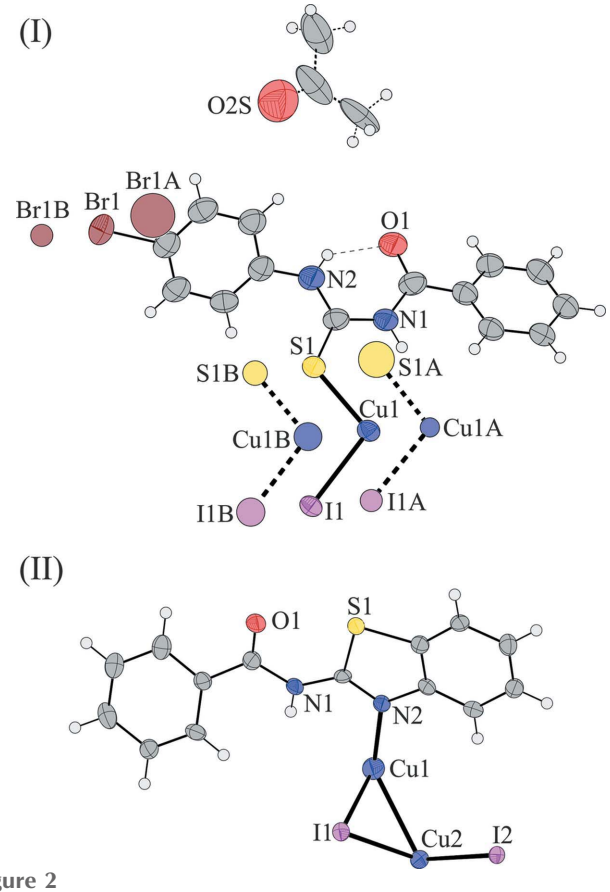

Figure 2
The asymmetric units of (I) and (II) with labels for the heteroatoms. Displacement ellipsoids are drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···I1^{i}	0.88	2.95	3.688 (6)	143
N2—H2···O1	0.88	1.92	2.635 (10)	137

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Table 3
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···I1^{i}	0.88	2.80	3.654 (10)	164

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

second and third disordered congeners is small (*ca* 4.5 and 5.5%, respectively; see Fig. 2). Moreover, the acetone molecule is located at a centre of inversion and is therefore disordered over two positions. There is a weak halogen interaction between bromine and the carbonyl oxygen of acetone [Br1···O2S^{i}; symmetry code: (i) $-x, -y, -z$], where the distance is 3.26 (2) Å.

Ignoring the Cu···Cu interactions, three iodide anions and one L^1 molecule are bonded to copper, forming a CuI_3S kernel that exhibits a slightly distorted tetrahedral geometry, with $\tau_4' = 0.90$ (Okuniewski *et al.*, 2015; see Fig. 3). The halogen atom (I1) serves as a bridging ligand connecting three Cu atoms. In this way, an infinite centrosymmetric chain of $_{\infty}\bar{1}$ rod group symmetry (*R*2; Kopský & Litvin, 2010), extended in the [100] direction, is formed (Fig. 4). The Cu···Cu contacts are not equal (see Fig. 3).

Compound (II) crystallizes in the monoclinic noncentrosymmetric space group $P2_1$. The lack of a point of inversion is due to the helicity of the polymeric chains. During synthesis, the L^2 ligand undergoes dehalogenation and cyclization to form *N*-(benzo[*d*]thiazol-2-yl)benzamide (L^{2c}), which can be found in the asymmetric unit connected *via* the N atom to two CuI units. The second N atom is involved in the only hydrogen bond present (see Table 3).

The benzothiazole fragment and carbonyl group are almost coplanar [dihedral angle 1.9 (5)°] and the phenyl group is inclined to the carbonyl group at an angle of 23.7 (6)°. Intramolecular S···O chalcogen interactions stabilize the planarity of the compound; the S1···O1 distance is 2.68 (1) Å. Such interactions are common in similar systems (Thomas *et al.*, 2015).

Omitting the Cu···Cu interactions, the first Cu atom (Cu1) forms a CuI_3N kernel that exhibits a distorted tetrahedral geometry, with $\tau_4' = 0.88$ (Fig. 3). The second Cu atom (Cu2) is located in the middle of the chain and forms a CuI_4 kernel. In this case, the geometry of the coordination centre is closer to ideal tetrahedral but is still slightly distorted ($\tau_4' = 0.90$). The halogen atoms (I1 and I2) serve as bridging ligands, connecting three or four Cu atoms, respectively. In that way, an infinite chiral chain with screw-axis symmetry ($_{\infty}112_1$; *R*9) is formed and propagates in the [010] direction (Fig. 4). The main bond lengths and Cu···Cu contact distances are depicted in Fig. 3.

The structure is stabilized by classical phenyl–phenyl and benzothiazoyl–benzothiazoyl π-stacking interactions, with the distance between ring centroids equal to the *b*-cell parameter [4.1152 (4) Å] and a slippage of 2.10 (2) Å. Additional weak

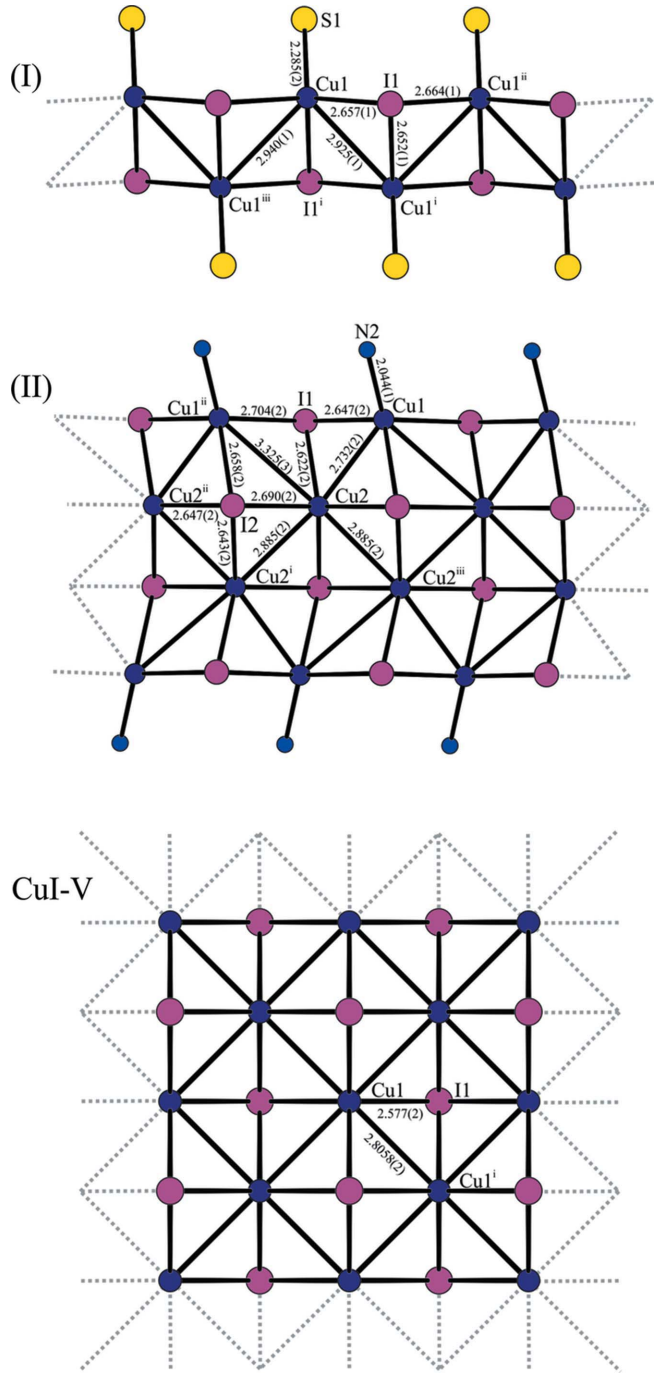

Figure 3
Coordination centres for (I), (II) and phase V copper iodide (*i.e.* CuI-V). Structural parameters and symmetry operations for (I): τ_4'(Cu1) = 0.90; (i) $-x+2, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x+1, -y+1, -z+1$; for (II): τ_4'(Cu1) = 0.88; τ_4'(Cu2) = 0.90; (i) $-x+2, y+\frac{1}{2}, -z+1$; (ii) $x, y+1, z$; (iii) $-x+2, y-\frac{1}{2}, -z+1$; for CuI-V: τ_4'(Cu1) = 0.94; (i) $y+\frac{1}{2}, -x+\frac{1}{2}, z$. Disorder of the main chain in (I) has been omitted for clarity.

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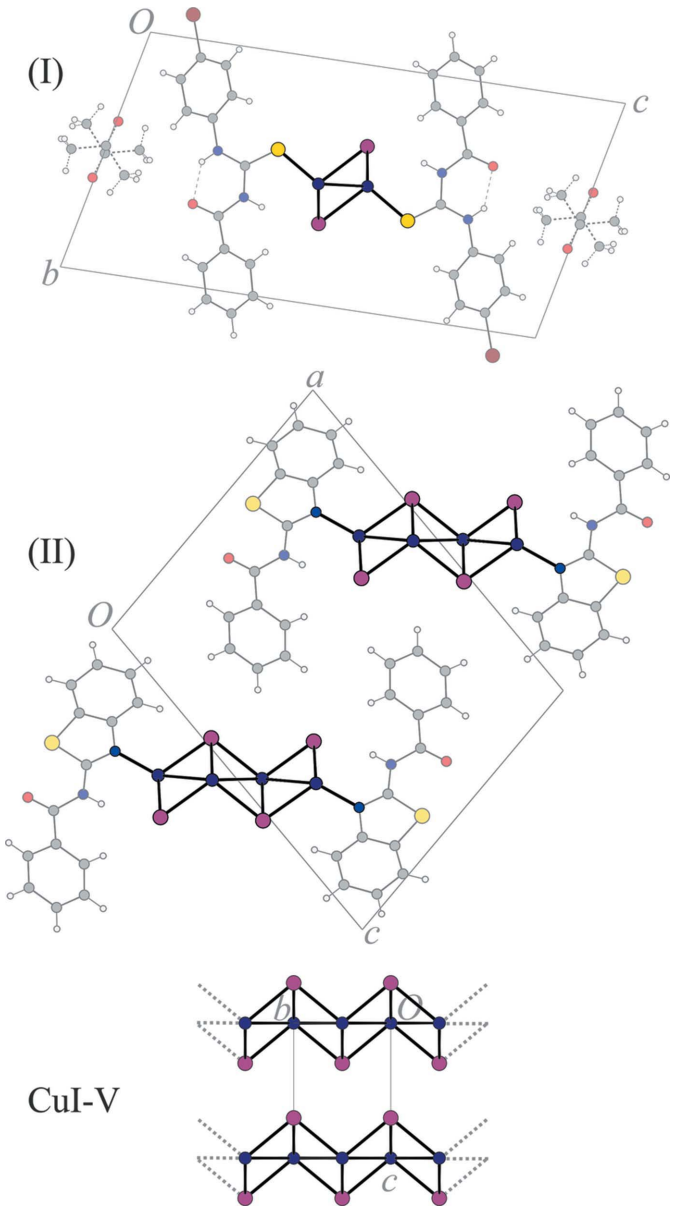

Figure 4
Packing diagrams for (I) and (II), viewed in the direction of the ribbon extension. Inorganic CuI fragments are emphasized. Disorder of the main chain in (I) has been omitted for clarity. For comparison, the packing diagram for phase V copper iodide (*i.e.* CuI-V) is shown at the bottom.

S···O, C—H···O and C—H···I interactions between ribbons allow the formation of a stable crystal structure.

4. Conclusions

Two copper(I) iodide coordination compounds with thiourea-related ligands have been prepared and structurally characterized. Both complexes are hybrid inorganic chains in the form of ribbons with a $(CuI)_n$ kernel, where close Cu···Cu contacts stabilized by the coordinated ligands can be found. Reported Cu···Cu distances are in the range 2.732 (2)–3.325 (3) Å and are close to the sum of the copper covalent radii [2.64 (8) Å; Cordero *et al.*, 2008].

During the synthesis of (I), L^1 remained unchanged and serves as an *S*-donor ligand. In contrast, during the synthesis of (II), L^2 was dehalogenated and cyclized to form the L^{2c} *N*-donor ligand. The two polymers crystallize in different space groups and the ribbons exhibit different rod-group symmetry, *i.e.* for (I), with inversion centres, and for (II), with a screw axis. In both cases, $(CuI)_n$ ribbons are formed, but in the structure of (I), they are arranged into a double chain and in (II) into a quadruple chain. Such ribbons can be considered as distorted fragments of CuI layers extracted from high-pressure phase V of copper(I) iodide (Hull & Keen, 1994; Figs. 3 and 4). Between ribbons, there are only weak dispersion interactions that stabilize the crystal structures (absence of strong intermolecular hydrogen bonds or ionic interactions).

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Copper(I) iodide ribbons coordinated with thiourea derivatives

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Computing details

For both structures, data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA* (Stoe & Cie, 2009); data reduction: *X-RED32* (Stoe & Cie, 2009); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Poly[[[1-benzoyl-3-(4-bromophenyl)thiourea-κS]-μ_3-iodido-copper(I)] acetone hemisolvate] (I)

Crystal data

$[CuBrI(C_{14}H_{11}N_2OS)]\cdot 0.5C_3H_6O$
M_r = 554.70
Triclinic, $P\overline{1}$
a = 4.0594 (3) Å
b = 10.8684 (8) Å
c = 20.7336 (15) Å
α = 102.079 (6)°
β = 94.047 (6)°
γ = 94.299 (6)°
V = 888.48 (11) Å^3
Z = 2
F(000) = 532
D_x = 2.073 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6948 reflections
θ = 2.5–29.5°
μ = 5.34 mm^{-1}
T = 120 K
Needle, colourless
0.44 × 0.02 × 0.02 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: microfocus sealed X-ray tube, GeniX Mo, 0.05 x 0.05 mm2
Parabolic x-ray mirror monochromator
rotation method scans
Absorption correction: integration [X-RED32 (Stoe & Cie, 2009), by Gaussian integration, analogous to Coppens (1970)]
T_{min} = 0.358, T_{max} = 0.905
7687 measured reflections
3446 independent reflections
3069 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 26.0°, θ_{min} = 2.5°
$h = -4 \rightarrow 5$
$k = -12 \rightarrow 13$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.175
S = 1.07
3446 reflections
257 parameters
40 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1209P)^2 + 2.3538P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 1.89 e Å^{-3}
$\Delta\rho_{min}$ = −2.96 e Å^{-3}

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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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.7353 (2)	0.50967 (9)	0.45015 (4)	0.0367 (3)	0.900 (2)
I1	0.72245 (10)	0.32964 (4)	0.51899 (2)	0.0331 (2)	0.900 (2)
Br1	0.3217 (2)	−0.09639 (9)	0.07159 (5)	0.0580 (3)	0.900 (2)
S1	0.6415 (5)	0.39525 (19)	0.34375 (9)	0.0395 (4)	0.900 (2)
Cu1A	0.785 (4)	0.6685 (15)	0.4747 (8)	0.029 (4)*	0.0453 (18)
I1A	0.776 (3)	0.4872 (10)	0.5400 (5)	0.038 (3)*	0.0453 (18)
Br1A	0.338 (15)	0.041 (6)	0.078 (3)	0.151 (18)*	0.0453 (18)
S1A	0.68 (2)	0.558 (9)	0.364 (5)	0.10 (2)*	0.0453 (18)
Cu1B	0.678 (5)	0.351 (2)	0.4294 (10)	0.060 (5)*	0.0551 (18)
I1B	0.666 (3)	0.1721 (12)	0.4984 (6)	0.062 (3)*	0.0551 (18)
Br1B	0.250 (3)	−0.2533 (12)	0.0517 (6)	0.038 (3)*	0.0551 (18)
S1B	0.583 (9)	0.241 (3)	0.3243 (18)	0.047 (8)*	0.0551 (18)
N1	0.8582 (17)	0.6097 (6)	0.3122 (3)	0.0463 (14)	
H1	0.860628	0.638312	0.355249	0.056*	
N2	0.7669 (19)	0.4367 (7)	0.2243 (3)	0.0522 (16)	
H2	0.832923	0.490828	0.200671	0.063*	
O1	0.967 (2)	0.6685 (6)	0.2156 (3)	0.0693 (19)	
C1	0.7634 (19)	0.4798 (8)	0.2899 (3)	0.0437 (16)	
C16	0.8901 (19)	0.8737 (7)	0.3752 (4)	0.0448 (16)	
H16	0.775127	0.815977	0.396345	0.054*	
C23	0.685 (2)	0.0867 (9)	0.1746 (4)	0.0531 (19)	
H23	0.762630	0.015384	0.188674	0.064*	
C10	0.948 (2)	0.6993 (9)	0.2763 (4)	0.0525 (19)	
C15	0.944 (2)	1.0023 (8)	0.4061 (4)	0.0466 (17)	
H15	0.858246	1.032465	0.447361	0.056*	
C25	0.362 (2)	0.1708 (9)	0.0960 (4)	0.057 (2)	
H25	0.220284	0.157117	0.056229	0.068*	
C21	0.670 (2)	0.3085 (8)	0.1901 (4)	0.0479 (18)	
C11	1.0076 (19)	0.8305 (8)	0.3129 (4)	0.0459 (16)	
C22	0.786 (2)	0.2072 (8)	0.2109 (4)	0.0485 (18)	
H22	0.933850	0.219393	0.249789	0.058*	
C24	0.474 (2)	0.0701 (9)	0.1188 (4)	0.0522 (19)	
C12	1.183 (2)	0.9161 (8)	0.2840 (4)	0.0474 (17)	
H12	1.264643	0.887651	0.242164	0.057*	
C13	1.239 (2)	1.0424 (8)	0.3152 (4)	0.0496 (18)	
H13	1.360063	1.099932	0.294903	0.060*	
C14	1.120 (2)	1.0847 (8)	0.3762 (4)	0.0484 (17)	
H14	1.160847	1.171341	0.397616	0.058*	
C26	0.460 (2)	0.2948 (9)	0.1323 (4)	0.056 (2)	

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H26	0.384693	0.366188	0.117945	0.067*	
O1S	−0.072 (7)	0.3846 (16)	0.0058 (12)	0.142 (7)	0.5
C2S	0.030 (5)	0.4885 (15)	0.0000 (8)	0.120 (7)	0.5
C3S	0.060 (9)	0.521 (2)	−0.0666 (9)	0.118 (8)	0.5
H3SA	−0.156737	0.502748	−0.092409	0.177*	0.5
H3SB	0.221112	0.469917	−0.090205	0.177*	0.5
H3SC	0.133864	0.610672	−0.060622	0.177*	0.5
C1S	0.128 (9)	0.5950 (18)	0.0589 (10)	0.120 (8)	0.5
H1SA	0.329045	0.577161	0.083131	0.180*	0.5
H1SB	−0.052060	0.603279	0.088163	0.180*	0.5
H1SC	0.171456	0.673967	0.043958	0.180*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0381 (5)	0.0382 (5)	0.0369 (5)	0.0022 (4)	0.0088 (4)	0.0139 (4)
I1	0.0297 (3)	0.0363 (3)	0.0374 (3)	0.00253 (18)	0.00804 (18)	0.0156 (2)
Br1	0.0554 (6)	0.0520 (6)	0.0599 (6)	−0.0024 (4)	0.0080 (4)	−0.0020 (4)
S1	0.0471 (11)	0.0387 (10)	0.0353 (9)	−0.0027 (8)	0.0116 (7)	0.0132 (7)
N1	0.056 (4)	0.046 (4)	0.038 (3)	−0.001 (3)	0.007 (3)	0.015 (3)
N2	0.063 (4)	0.052 (4)	0.043 (3)	−0.004 (3)	0.015 (3)	0.015 (3)
O1	0.107 (6)	0.058 (4)	0.045 (3)	−0.007 (4)	0.017 (3)	0.021 (3)
C1	0.045 (4)	0.051 (4)	0.036 (3)	−0.002 (3)	0.006 (3)	0.013 (3)
C16	0.046 (4)	0.045 (4)	0.046 (4)	0.000 (3)	0.006 (3)	0.019 (3)
C23	0.056 (5)	0.063 (5)	0.041 (4)	0.001 (4)	0.018 (3)	0.009 (4)
C10	0.059 (5)	0.061 (5)	0.038 (4)	0.002 (4)	0.009 (3)	0.012 (3)
C15	0.048 (4)	0.050 (4)	0.046 (4)	0.009 (3)	0.005 (3)	0.019 (3)
C25	0.054 (5)	0.070 (6)	0.045 (4)	−0.005 (4)	0.008 (3)	0.011 (4)
C21	0.050 (4)	0.052 (5)	0.042 (4)	0.000 (3)	0.015 (3)	0.008 (3)
C11	0.045 (4)	0.047 (4)	0.048 (4)	0.000 (3)	0.003 (3)	0.018 (3)
C22	0.049 (4)	0.061 (5)	0.039 (4)	0.002 (4)	0.011 (3)	0.017 (3)
C24	0.054 (5)	0.058 (5)	0.044 (4)	−0.002 (4)	0.015 (3)	0.007 (4)
C12	0.046 (4)	0.055 (5)	0.043 (4)	0.001 (3)	0.010 (3)	0.016 (3)
C13	0.042 (4)	0.054 (5)	0.059 (5)	0.003 (3)	0.009 (3)	0.025 (4)
C14	0.048 (4)	0.048 (4)	0.053 (4)	0.002 (3)	0.005 (3)	0.018 (3)
C26	0.061 (5)	0.059 (5)	0.047 (4)	0.003 (4)	0.010 (4)	0.012 (4)
O1S	0.173 (18)	0.124 (14)	0.127 (15)	−0.001 (15)	0.022 (14)	0.023 (12)
C2S	0.144 (16)	0.086 (12)	0.158 (15)	0.034 (12)	0.027 (13)	0.078 (11)
C3S	0.15 (2)	0.069 (13)	0.151 (18)	0.020 (14)	0.040 (17)	0.049 (13)
C1S	0.15 (2)	0.098 (14)	0.141 (17)	0.028 (15)	0.020 (16)	0.095 (12)

Geometric parameters (Å, º)

Cu1—Cu1^{i}	2.9257 (19)	C23—C22	1.384 (12)
Cu1—Cu1^{ii}	2.9402 (18)	C23—C24	1.362 (13)
Cu1—I1^{ii}	2.6643 (10)	C10—C11	1.462 (12)
Cu1—I1	2.6520 (10)	C15—H15	0.9500
Cu1—I1^{i}	2.6576 (11)	C15—C14	1.377 (11)

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Cu1—S1	2.285 (2)	C25—H25	0.9500
Br1—C24	1.903 (9)	C25—C24	1.374 (14)
S1—C1	1.666 (7)	C25—C26	1.411 (13)
Cu1A—I1A^{ii}	2.69 (2)	C21—C22	1.366 (12)
Cu1A—I1A	2.614 (18)	C21—C26	1.398 (12)
Cu1A—I1A^{i}	2.540 (19)	C11—C12	1.387 (11)
Cu1A—S1A	2.35 (9)	C22—H22	0.9500
I1A—I1A^{i}	2.59 (2)	C12—H12	0.9500
I1A—I1A^{ii}	2.76 (2)	C12—C13	1.384 (12)
Cu1B—I1B	2.64 (2)	C13—H13	0.9500
Cu1B—S1B	2.25 (4)	C13—C14	1.386 (12)
N1—H1	0.8800	C14—H14	0.9500
N1—C1	1.405 (10)	C26—H26	0.9500
N1—C10	1.388 (11)	O1S—C2S	1.2070
N2—H2	0.8800	C2S—C3S	1.5042
N2—C1	1.343 (10)	C2S—C1S	1.5040
N2—C21	1.436 (10)	C3S—H3SA	0.9800
O1—C10	1.242 (10)	C3S—H3SB	0.9800
C16—H16	0.9500	C3S—H3SC	0.9800
C16—C15	1.404 (11)	C1S—H1SA	0.9800
C16—C11	1.408 (11)	C1S—H1SB	0.9800
C23—H23	0.9500	C1S—H1SC	0.9800

Cu1^{i}—Cu1—Cu1^{ii}	87.58 (5)	C14—C15—C16	119.8 (7)
I1—Cu1—Cu1^{i}	56.65 (3)	C14—C15—H15	120.1
I1^{i}—Cu1—Cu1^{ii}	120.17 (5)	C24—C25—H25	120.3
I1^{ii}—Cu1—Cu1^{ii}	56.22 (3)	C24—C25—C26	119.4 (8)
I1^{i}—Cu1—Cu1^{i}	56.47 (3)	C26—C25—H25	120.3
I1^{ii}—Cu1—Cu1^{i}	120.04 (5)	C22—C21—N2	122.7 (7)
I1—Cu1—Cu1^{ii}	56.62 (3)	C22—C21—C26	122.2 (8)
I1—Cu1—I1^{i}	113.12 (4)	C26—C21—N2	115.1 (8)
I1—Cu1—I1^{ii}	112.84 (3)	C16—C11—C10	123.0 (7)
I1^{i}—Cu1—I1^{ii}	99.42 (3)	C12—C11—C16	119.0 (7)
S1—Cu1—Cu1^{ii}	121.97 (7)	C12—C11—C10	118.0 (7)
S1—Cu1—Cu1^{i}	127.74 (8)	C23—C22—H22	120.4
S1—Cu1—I1^{i}	117.82 (6)	C21—C22—C23	119.1 (8)
S1—Cu1—I1^{ii}	112.19 (7)	C21—C22—H22	120.4
S1—Cu1—I1	101.98 (6)	C23—C24—Br1	119.6 (7)
Cu1^{i}—I1—Cu1^{ii}	99.42 (3)	C23—C24—C25	121.7 (9)
Cu1—I1—Cu1^{i}	66.88 (4)	C25—C24—Br1	118.7 (7)
Cu1—I1—Cu1^{ii}	67.15 (3)	C11—C12—H12	119.6
C1—S1—Cu1	111.3 (3)	C13—C12—C11	120.9 (7)
I1A^{i}—Cu1A—I1A	60.3 (5)	C13—C12—H12	119.6
S1A—Cu1A—I1A^{i}	76 (2)	C12—C13—H13	120.0
S1A—Cu1A—I1A	103 (2)	C12—C13—C14	119.9 (8)
Cu1A^{i}—I1A—Cu1A	119.7 (5)	C14—C13—H13	120.0
Cu1A^{i}—I1A—I1A^{i}	61.3 (6)	C15—C14—C13	120.6 (8)
I1A^{i}—I1A—Cu1A	58.4 (5)	C15—C14—H14	119.7

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S1B—Cu1B—I1B	102.9 (13)	C13—C14—H14	119.7
C1—N1—H1	115.3	C25—C26—H26	121.3
C10—N1—H1	115.3	C21—C26—C25	117.5 (9)
C10—N1—C1	129.4 (6)	C21—C26—H26	121.3
C1—N2—H2	117.7	O1S—C2S—C3S	122.2
C1—N2—C21	124.6 (7)	O1S—C2S—C1S	122.0
C21—N2—H2	117.7	C1S—C2S—C3S	115.8
N1—C1—S1	119.3 (5)	C2S—C3S—H3SA	109.5
N2—C1—S1	125.9 (6)	C2S—C3S—H3SB	109.5
N2—C1—N1	114.7 (7)	C2S—C3S—H3SC	109.5
C15—C16—H16	120.1	H3SA—C3S—H3SB	109.5
C15—C16—C11	119.7 (7)	H3SA—C3S—H3SC	109.5
C11—C16—H16	120.1	H3SB—C3S—H3SC	109.5
C22—C23—H23	120.0	C2S—C1S—H1SA	109.5
C24—C23—H23	120.0	C2S—C1S—H1SB	109.5
C24—C23—C22	120.1 (9)	C2S—C1S—H1SC	109.5
N1—C10—C11	116.8 (7)	H1SA—C1S—H1SB	109.5
O1—C10—N1	120.8 (8)	H1SA—C1S—H1SC	109.5
O1—C10—C11	122.3 (8)	H1SB—C1S—H1SC	109.5
C16—C15—H15	120.1		

Cu1—S1—C1—N1	−9.1 (7)	C10—C11—C12—C13	178.3 (8)
Cu1—S1—C1—N2	174.3 (6)	C15—C16—C11—C10	−177.1 (8)
N1—C10—C11—C16	−18.5 (12)	C15—C16—C11—C12	1.7 (11)
N1—C10—C11—C12	162.6 (8)	C21—N2—C1—S1	−1.2 (12)
N2—C21—C22—C23	−179.0 (7)	C21—N2—C1—N1	−178.1 (7)
N2—C21—C26—C25	178.8 (7)	C11—C16—C15—C14	−2.2 (12)
O1—C10—C11—C16	159.2 (9)	C11—C12—C13—C14	−0.1 (12)
O1—C10—C11—C12	−19.6 (13)	C22—C23—C24—Br1	−177.2 (6)
C1—N1—C10—O1	−2.9 (15)	C22—C23—C24—C25	1.5 (13)
C1—N1—C10—C11	174.8 (8)	C22—C21—C26—C25	1.3 (12)
C1—N2—C21—C22	−48.9 (12)	C24—C23—C22—C21	0.3 (12)
C1—N2—C21—C26	133.6 (9)	C24—C25—C26—C21	0.5 (12)
C16—C15—C14—C13	1.5 (12)	C12—C13—C14—C15	−0.3 (12)
C16—C11—C12—C13	−0.6 (12)	C26—C25—C24—Br1	176.8 (6)
C10—N1—C1—S1	−175.8 (7)	C26—C25—C24—C23	−1.9 (13)
C10—N1—C1—N2	1.2 (12)	C26—C21—C22—C23	−1.7 (12)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···I1^{i}	0.88	2.95	3.688 (6)	143
N2—H2···O1	0.88	1.92	2.635 (10)	137

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

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Poly[μ_4-iodido-μ_3-iodido-[*N*-(benzo[*d*]thiazol-2-yl)benzamide-κN]dicopper(I)] (II)

Crystal data

$[Cu_2I_2(C_{14}H_{10}N_2OS)]$
M_r = 635.18
Monoclinic, $P2_1$
a = 12.6880 (12) Å
b = 4.1152 (4) Å
c = 15.8952 (15) Å
β = 100.258 (8)°
V = 816.68 (14) Å^3
Z = 2
$F(000)$ = 592
D_x = 2.583 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1069 reflections
θ = 2.9–29.4°
μ = 6.51 mm^{-1}
T = 120 K
Needle, brown
0.57 × 0.09 × 0.06 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: microfocus sealed X-ray tube, GeniX Mo, 0.05 x 0.05 mm2
Parabolic x-ray mirror monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration [X-RED32 (Stoe & Cie, 2009), by Gaussian integration, analogous to Coppens (1970)]
T_{min} = 0.175, T_{max} = 0.688
7646 measured reflections
3163 independent reflections
3139 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.0°, θ_{min} = 2.6°
$h = -15 \rightarrow 15$
$k = -4 \rightarrow 5$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.121
S = 1.06
3163 reflections
199 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0771P)^2 + 6.6934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.31 e Å^{-3}
$\Delta\rho_{min}$ = −2.03 e Å^{-3}
Absolute structure: Flack x determined using 1322 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.11 (6)

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_{iso}*/U_{eq}
I2	1.02099 (5)	0.89173 (17)	0.37962 (5)	0.0200 (2)
I1	0.72945 (6)	0.48198 (19)	0.41104 (5)	0.0220 (2)
Cu2	0.93650 (12)	0.3849 (4)	0.45145 (10)	0.0270 (4)
Cu1	0.81130 (14)	−0.0090 (5)	0.33639 (12)	0.0373 (4)
S1	0.6135 (2)	0.1705 (8)	0.07118 (19)	0.0233 (6)
O1	0.4394 (7)	−0.107 (3)	0.1140 (5)	0.031 (2)
N1	0.5840 (8)	−0.123 (3)	0.2190 (6)	0.024 (2)

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H1	0.609540	−0.193974	0.270900	0.028*
N2	0.7534 (8)	0.087 (3)	0.2105 (6)	0.021 (2)
C1	0.6534 (9)	0.030 (3)	0.1759 (7)	0.020 (2)
C25	0.9109 (9)	0.371 (4)	0.1740 (7)	0.024 (2)
H25	0.953311	0.330248	0.228530	0.029*
C21	0.7436 (10)	0.325 (3)	0.0755 (8)	0.023 (2)
C22	0.7821 (9)	0.498 (4)	0.0125 (8)	0.026 (3)
H22	0.737748	0.543116	−0.040998	0.031*
C13	0.2541 (10)	−0.612 (4)	0.2674 (9)	0.036 (3)
H13	0.190294	−0.725404	0.243961	0.044*
C10	0.4763 (10)	−0.176 (4)	0.1874 (8)	0.026 (3)
C24	0.9525 (10)	0.544 (4)	0.1116 (8)	0.027 (3)
H24	1.024029	0.622134	0.123787	0.033*
C14	0.2820 (11)	−0.581 (4)	0.3551 (9)	0.037 (3)
H14	0.238052	−0.671896	0.391680	0.044*
C20	0.8073 (9)	0.263 (3)	0.1545 (7)	0.021 (2)
C11	0.4125 (9)	−0.319 (3)	0.2479 (8)	0.025 (3)
C12	0.3176 (10)	−0.481 (4)	0.2121 (10)	0.033 (3)
H12	0.297025	−0.501082	0.151884	0.040*
C23	0.8890 (10)	0.604 (4)	0.0305 (9)	0.029 (3)
H23	0.918855	0.715912	−0.011950	0.035*
C15	0.3770 (10)	−0.413 (4)	0.3895 (8)	0.033 (3)
H15	0.396217	−0.386533	0.449633	0.040*
C16	0.4414 (10)	−0.287 (4)	0.3374 (8)	0.028 (3)
H16	0.505710	−0.177906	0.361500	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I2	0.0181 (3)	0.0203 (4)	0.0216 (4)	0.0004 (3)	0.0039 (3)	0.0007 (3)
I1	0.0204 (4)	0.0224 (4)	0.0231 (4)	0.0016 (3)	0.0034 (3)	0.0030 (3)
Cu2	0.0247 (7)	0.0292 (9)	0.0271 (7)	−0.0026 (7)	0.0049 (6)	−0.0040 (7)
Cu1	0.0349 (8)	0.0414 (11)	0.0348 (9)	−0.0009 (9)	0.0046 (7)	0.0011 (9)
S1	0.0187 (13)	0.0324 (17)	0.0183 (13)	0.0016 (12)	0.0019 (10)	0.0030 (12)
O1	0.026 (4)	0.047 (6)	0.020 (4)	0.001 (5)	0.002 (3)	0.005 (5)
N1	0.022 (4)	0.033 (6)	0.016 (4)	0.001 (5)	0.003 (4)	0.003 (5)
N2	0.022 (5)	0.024 (5)	0.017 (5)	0.000 (4)	0.003 (4)	0.004 (4)
C1	0.017 (5)	0.028 (7)	0.014 (5)	0.003 (5)	−0.001 (4)	−0.002 (5)
C25	0.028 (6)	0.025 (6)	0.019 (5)	0.003 (5)	0.004 (4)	−0.002 (5)
C21	0.024 (5)	0.022 (7)	0.025 (6)	0.002 (5)	0.006 (4)	−0.002 (5)
C22	0.021 (5)	0.037 (7)	0.018 (5)	0.002 (6)	−0.001 (4)	0.001 (6)
C13	0.026 (6)	0.039 (8)	0.044 (8)	−0.001 (6)	0.007 (6)	0.005 (7)
C10	0.024 (6)	0.025 (7)	0.029 (6)	0.001 (5)	0.007 (5)	−0.005 (5)
C24	0.024 (6)	0.025 (7)	0.033 (7)	−0.001 (5)	0.008 (5)	−0.007 (6)
C14	0.030 (6)	0.046 (10)	0.038 (7)	0.006 (7)	0.013 (6)	0.015 (7)
C20	0.023 (5)	0.022 (6)	0.020 (6)	0.003 (5)	0.007 (4)	−0.002 (5)
C11	0.021 (5)	0.029 (7)	0.025 (6)	0.004 (5)	0.006 (5)	−0.004 (5)
C12	0.026 (6)	0.030 (7)	0.044 (8)	0.002 (6)	0.008 (6)	0.003 (7)

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C23	0.023 (6)	0.035 (8)	0.030 (7)	0.001 (6)	0.006 (5)	0.005 (6)
C15	0.024 (6)	0.050 (9)	0.025 (6)	−0.003 (6)	0.002 (5)	0.003 (6)
C16	0.028 (6)	0.037 (8)	0.019 (6)	0.006 (6)	0.004 (5)	−0.004 (5)

Geometric parameters (Å, º)

I2—Cu2^{i}	2.6431 (18)	C25—C20	1.370 (17)
I2—Cu2	2.6905 (18)	C21—C22	1.386 (18)
I2—Cu2^{ii}	2.6473 (18)	C21—C20	1.392 (17)
I2—Cu1^{ii}	2.658 (2)	C22—H22	0.9500
I1—Cu2	2.6216 (17)	C22—C23	1.406 (17)
I1—Cu1^{ii}	2.704 (2)	C13—H13	0.9500
I1—Cu1	2.647 (2)	C13—C14	1.38 (2)
Cu2—Cu2^{iii}	2.885 (2)	C13—C12	1.403 (19)
Cu2—Cu2^{i}	2.885 (2)	C10—C11	1.485 (17)
Cu2—Cu1	2.732 (2)	C24—H24	0.9500
Cu1—N2	2.044 (10)	C24—C23	1.414 (19)
S1—C1	1.749 (11)	C14—H14	0.9500
S1—C21	1.759 (13)	C14—C15	1.41 (2)
O1—C10	1.210 (16)	C11—C12	1.406 (19)
N1—H1	0.8800	C11—C16	1.411 (17)
N1—C1	1.363 (16)	C12—H12	0.9500
N1—C10	1.387 (15)	C23—H23	0.9500
N2—C1	1.311 (15)	C15—H15	0.9500
N2—C20	1.414 (15)	C15—C16	1.364 (19)
C25—H25	0.9500	C16—H16	0.9500
C25—C24	1.398 (18)		
Cu2^{i}—I2—Cu2^{ii}	66.11 (5)	C1—N2—C20	111.6 (10)
Cu2^{ii}—I2—Cu2	100.88 (5)	C20—N2—Cu1	125.8 (8)
Cu2^{i}—I2—Cu2	65.50 (5)	N1—C1—S1	121.9 (8)
Cu2^{i}—I2—Cu1^{ii}	106.14 (6)	N2—C1—S1	115.7 (9)
Cu2^{ii}—I2—Cu1^{ii}	61.97 (6)	N2—C1—N1	122.3 (10)
Cu1^{ii}—I2—Cu2	76.87 (6)	C24—C25—H25	120.9
Cu2—I1—Cu1	62.45 (6)	C20—C25—H25	120.9
Cu2—I1—Cu1^{ii}	77.24 (6)	C20—C25—C24	118.2 (11)
Cu1—I1—Cu1^{ii}	100.52 (6)	C22—C21—S1	127.4 (10)
I2^{iii}—Cu2—I2^{iv}	114.92 (7)	C22—C21—C20	121.6 (11)
I2^{iii}—Cu2—I2	113.47 (6)	C20—C21—S1	111.0 (9)
I2^{iv}—Cu2—I2	100.88 (5)	C21—C22—H22	121.2
I2^{iv}—Cu2—Cu2^{i}	123.16 (8)	C21—C22—C23	117.6 (11)
I2^{iii}—Cu2—Cu2^{iii}	58.04 (6)	C23—C22—H22	121.2
I2—Cu2—Cu2^{i}	56.46 (4)	C14—C13—H13	119.2
I2^{iii}—Cu2—Cu2^{i}	57.02 (6)	C14—C13—C12	121.6 (14)
I2^{iv}—Cu2—Cu2^{iii}	56.88 (4)	C12—C13—H13	119.2
I2—Cu2—Cu2^{iii}	123.57 (8)	O1—C10—N1	120.0 (12)
I2—Cu2—Cu1	113.83 (7)	O1—C10—C11	123.8 (11)
I2^{iv}—Cu2—Cu1	59.21 (5)	N1—C10—C11	116.2 (11)

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I2^{iii}—Cu2—Cu1	132.51 (8)	C25—C24—H24	119.7
I1—Cu2—I2	103.62 (6)	C25—C24—C23	120.7 (12)
I1—Cu2—I2^{iii}	105.17 (6)	C23—C24—H24	119.7
I1—Cu2—I2^{iv}	118.44 (6)	C13—C14—H14	120.6
I1—Cu2—Cu2^{iii}	132.81 (7)	C13—C14—C15	118.9 (13)
I1—Cu2—Cu2^{i}	117.53 (6)	C15—C14—H14	120.6
I1—Cu2—Cu1	59.23 (6)	C25—C20—N2	125.2 (11)
Cu2^{iii}—Cu2—Cu2^{i}	90.97 (9)	C25—C20—C21	121.6 (11)
Cu1—Cu2—Cu2^{i}	169.75 (8)	C21—C20—N2	113.2 (10)
Cu1—Cu2—Cu2^{iii}	97.92 (5)	C12—C11—C10	116.9 (11)
I2^{iv}—Cu1—I1^{iv}	102.26 (7)	C12—C11—C16	120.2 (12)
I2^{iv}—Cu1—Cu2	58.81 (5)	C16—C11—C10	122.9 (12)
I1—Cu1—I2^{iv}	117.13 (7)	C13—C12—C11	118.4 (13)
I1—Cu1—I1^{iv}	100.52 (6)	C13—C12—H12	120.8
I1^{iv}—Cu1—Cu2	112.88 (7)	C11—C12—H12	120.8
I1—Cu1—Cu2	58.32 (5)	C22—C23—C24	120.3 (12)
N2—Cu1—I2^{iv}	116.8 (3)	C22—C23—H23	119.9
N2—Cu1—I1^{iv}	118.7 (3)	C24—C23—H23	119.9
N2—Cu1—I1	100.9 (3)	C14—C15—H15	119.5
N2—Cu1—Cu2	127.3 (3)	C16—C15—C14	120.9 (13)
C1—S1—C21	88.4 (6)	C16—C15—H15	119.5
C1—N1—H1	117.5	C11—C16—H16	120.0
C1—N1—C10	124.9 (10)	C15—C16—C11	120.0 (13)
C10—N1—H1	117.5	C15—C16—H16	120.0
C1—N2—Cu1	121.9 (8)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···I1^{iv}	0.88	2.80	3.654 (10)	164

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

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