

Poly[tetra- $\mu_{1,1}$ -azido-bis(μ_2 -pyrimidine-2-carboxylato)tricopper(II)]

Jiong-Peng Zhao and Fu-Chen Liu*

School of Chemistry and Chemical Engineering, Tianjin University of Technology, Tianjin 300191, People's Republic of China
Correspondence e-mail: fuchenliu@yaho.com

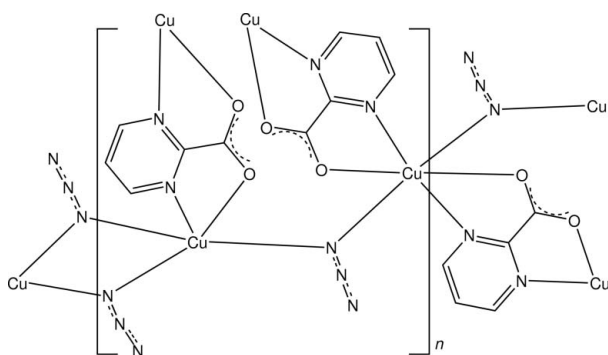
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.011$ Å; R factor = 0.052; wR factor = 0.134; data-to-parameter ratio = 10.4.

In the title compound, $[\text{Cu}_3(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{N}_3)_4]_n$, one of the Cu^{II} atoms lies on an inversion centre and is octahedrally coordinated by two bidentate chelating pyrimidine-2-carboxylate ligands and two azide anions, each of which gives an $N:N$ -bridge to the second inversion-related Cu^{II} centre in the formula unit. The second Cu^{II} atom is five-coordinated with a distorted square-pyramidal coordination sphere comprising a single bidentate chelating pyrimidine-2-carboxylate anion and three azide N anions, two of which doubly bridge centrosymmetric Cu^{II} centres, giving a two-dimensional network structure extending parallel to (010).

Related literature

Copper azide complexes have attracted much attention in recent years because the azide anions can mediate magnetic interactions effectively between the copper ions, see: Zhao *et al.* (2009). The structures of the complexes are dependant on the co-ligand and conditions employed in the synthesis, see: Zeng *et al.* (2009). For azide complexes with 2,2'-bipyrimidine or oxalate as co-ligands, see: Cortes *et al.* (1996); Escuer *et al.* (1994) and for an azide complex with a pyrimidine-2-carboxylate ligand, see: Suarez-Varela *et al.* (2008).



Experimental

Crystal data

$[\text{Cu}_3(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{N}_3)_4]$
 $M_r = 604.96$
Monoclinic, $P2_1/c$
 $a = 7.4743$ (15) Å
 $b = 14.997$ (3) Å
 $c = 9.479$ (4) Å
 $\beta = 122.31$ (2)°

$V = 898.0$ (5) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 3.59$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.18 \times 0.18$ mm

Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\text{min}} = 0.625$, $T_{\text{max}} = 1.000$

7028 measured reflections
1572 independent reflections
1305 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.134$
 $S = 1.24$
1572 reflections

151 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Data collection: *SCXmini Benchtop Crystallography System Software* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2045).

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supplementary materials

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J.-P. Zhao and F.-C. Liu

Comment

Copper azide complexes have attracted much attention in recent years because the azide anions can mediate magnetic interactions effectively between the copper ions (Zhao *et al.*, 2009). The structures of those complexes are dependant on the co-ligand and conditions employed in the synthesis (Zeng *et al.*, 2009). Some azide complexes with 2,2'-bipyrimidine or oxalate as co-ligands have been reported (Cortes *et al.*, 1996); Escuer *et al.*, 1994). The pyrimidine-2-carboxylate ligand can be considered as the combination of 2,2'-bipyrimidine and oxalate, and a new metal azide complex with it as ligand has been reported (Suarez-Varela *et al.*, 2008). In this work we report a new copper(II) azide complex with pyrimidine-2-carboxylate as co-ligand, $[\text{Cu}_3(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{N}_3)_4]_n$ (I), prepared under hydrothermal conditions and its structure is reported here.

In the asymmetric units of the title compound, there are one and a half copper(II) cations, two azido anions and two pyrimidine-2-carboxylate ligands (Fig. 1). One of the cations (Cu2) lies on an inversion centre and is octahedrally coordinated by two bidentate chelate pyrimidine-2-carboxylato-N,O ligands and two azido anions, each giving an N bridge to the inversion-related Cu1 centres in the formula unit $[\text{Cu}_2\text{—Cu1}, 3.4652(14) \text{ \AA}]$. A second weak contact between a carboxyl O (O1) to Cu1 is also present $[\text{Cu1}\cdots\text{O1}, 2.950(4) \text{ \AA}]$ but is too long to be considered a bridging (Cu—O) bond. The coordination sphere about Cu1 is five-coordinate with a distorted square pyramidal coordination sphere comprising a single bidentate chelate pyrimidine-2-carboxylate anion and three azido N anions, one bridging to Cu2, the other two giving double N bridges to centrosymmetrically related Cu centres $[\text{Cu1—Cu1}^{\text{iii}}, 3.329(2) \text{ \AA}]$ [symmetry code: (iii) $x - 1, y, z$]. Structure extension results in a two-dimensional network (Figs. 2, 3).

Experimental

A mixture of copper(II) nitrate (1.5 mmol) and sodium azide (2 mmol), and pyrimidine-2-carboxylic acid (0.5 mmol) in 10 ml of water was sealed in a Teflon-lined stainless-steel Parr bomb that was heated at 413 K for 48 h. Black crystals of the title complex were collected after the bomb was allowed to cool to room temperature (yield 20% based on Cu). Caution: azides may be explosive: although we have had no problems in this work, only small quantities should be prepared and should be handled with great caution.

Refinement

Hydrogen atoms were included in calculated positions and treated as riding on their parent C atoms with $\text{C—H} = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

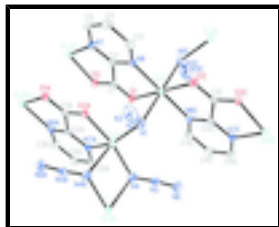


Fig. 1. The coordination mode and linkage of the metal ions and ligands in (I). Ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) $-x + 2, -y, -z$; (B) $-x + 1, -y, -z - 1$; (C) $-x + 1, -y, -z$; (D) $x - 1, y, z$].

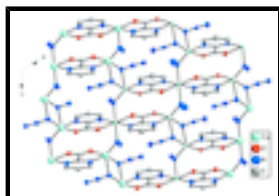


Fig. 2. The two-dimensional network structure of (I).

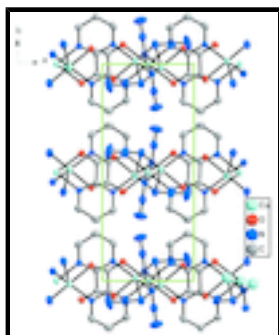


Fig. 3. The packing mode of the complex in the unit cell.

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Crystal data

$[\text{Cu}_3(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{N}_3)_4]$

$M_r = 604.96$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 7.4743\ (15)\ \text{\AA}$

$b = 14.997\ (3)\ \text{\AA}$

$c = 9.479\ (4)\ \text{\AA}$

$\beta = 122.31\ (2)^\circ$

$V = 898.0\ (5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 594$

$D_x = 2.237\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7433 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 3.59\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, black

$0.20 \times 0.18 \times 0.18\ \text{mm}$

Data collection

Rigaku SCXmini CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scans

1572 independent reflections

1305 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 3.2^\circ$

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.625$, $T_{\max} = 1.000$
7028 measured reflections

$h = -8 \rightarrow 8$
 $k = -17 \rightarrow 17$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.134$
 $S = 1.24$
1572 reflections
151 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 2.0516P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.71 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.64025 (11)	-0.01316 (5)	-0.29370 (10)	0.0259 (3)
Cu2	0.50000	0.00000	0.00000	0.0221 (3)
O1	0.7728 (6)	-0.0882 (3)	0.0359 (5)	0.0278 (12)
O2	1.1215 (6)	-0.0703 (3)	0.1528 (5)	0.0234 (12)
N1	0.4612 (8)	0.0444 (4)	-0.2223 (7)	0.0279 (17)
N2	0.4377 (9)	0.1253 (4)	-0.2455 (7)	0.0344 (19)
N3	0.4134 (13)	0.2001 (5)	-0.2695 (10)	0.063 (3)
N4	0.4241 (9)	-0.0895 (4)	-0.4673 (7)	0.0365 (19)
N5	0.2454 (9)	-0.0933 (4)	-0.4977 (6)	0.035 (2)
N6	0.0719 (11)	-0.0987 (6)	-0.5367 (8)	0.064 (3)
N7	1.1181 (8)	0.0896 (3)	0.2648 (6)	0.0245 (17)
N8	0.7462 (8)	0.0827 (3)	0.1309 (6)	0.0224 (17)
C1	0.9407 (9)	-0.0464 (4)	0.1173 (7)	0.0214 (17)
C2	0.9320 (9)	0.0481 (4)	0.1760 (7)	0.0221 (17)
C3	0.7414 (11)	0.1682 (4)	0.1722 (9)	0.033 (2)

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C4	0.9286 (12)	0.2167 (5)	0.2647 (9)	0.038 (3)
C5	1.1161 (11)	0.1746 (4)	0.3094 (8)	0.032 (2)
H3A	0.61250	0.19510	0.13880	0.0390*
H4A	0.92720	0.27550	0.29530	0.0460*
H5A	1.24310	0.20550	0.37130	0.0390*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0184 (4)	0.0326 (5)	0.0258 (5)	-0.0030 (3)	0.0112 (4)	-0.0039 (3)
Cu2	0.0168 (6)	0.0274 (6)	0.0215 (6)	-0.0014 (4)	0.0099 (5)	-0.0009 (4)
O1	0.026 (2)	0.026 (2)	0.030 (2)	-0.0038 (19)	0.014 (2)	-0.0047 (19)
O2	0.018 (2)	0.028 (2)	0.023 (2)	-0.0004 (17)	0.0102 (18)	-0.0010 (18)
N1	0.025 (3)	0.031 (3)	0.034 (3)	-0.001 (2)	0.020 (3)	0.001 (3)
N2	0.029 (3)	0.048 (4)	0.035 (3)	-0.001 (3)	0.023 (3)	-0.001 (3)
N3	0.091 (6)	0.032 (4)	0.092 (6)	0.014 (4)	0.066 (5)	0.011 (4)
N4	0.026 (3)	0.045 (4)	0.035 (3)	-0.003 (3)	0.014 (3)	-0.010 (3)
N5	0.035 (4)	0.050 (4)	0.018 (3)	-0.012 (3)	0.012 (3)	-0.002 (3)
N6	0.034 (4)	0.114 (7)	0.040 (4)	-0.025 (4)	0.018 (3)	-0.001 (4)
N7	0.021 (3)	0.024 (3)	0.026 (3)	-0.005 (2)	0.011 (2)	-0.003 (2)
N8	0.021 (3)	0.025 (3)	0.022 (3)	-0.001 (2)	0.012 (2)	-0.002 (2)
C1	0.021 (3)	0.026 (3)	0.016 (3)	-0.001 (3)	0.009 (3)	0.000 (3)
C2	0.027 (3)	0.020 (3)	0.022 (3)	0.000 (3)	0.015 (3)	0.002 (2)
C3	0.035 (4)	0.029 (4)	0.037 (4)	0.007 (3)	0.021 (3)	0.002 (3)
C4	0.047 (5)	0.025 (4)	0.041 (4)	0.000 (3)	0.022 (4)	-0.004 (3)
C5	0.030 (4)	0.035 (4)	0.026 (4)	-0.011 (3)	0.012 (3)	-0.004 (3)

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

Cu1—N1	1.991 (7)	N2—N3	1.140 (10)
Cu1—N4	1.946 (6)	N4—N5	1.208 (10)
Cu1—N4 ⁱ	2.563 (6)	N5—N6	1.146 (12)
Cu1—O2 ⁱⁱ	1.995 (5)	N7—C2	1.334 (9)
Cu1—N7 ⁱⁱ	2.030 (6)	N7—C5	1.346 (8)
Cu2—O1	2.298 (5)	N8—C2	1.321 (10)
Cu2—N1	2.077 (6)	N8—C3	1.347 (8)
Cu2—N8	2.006 (6)	C1—C2	1.537 (9)
Cu2—O1 ⁱⁱⁱ	2.298 (5)	C3—C4	1.394 (12)
Cu2—N1 ⁱⁱⁱ	2.077 (6)	C4—C5	1.381 (13)
Cu2—N8 ⁱⁱⁱ	2.006 (5)	C3—H3A	0.9300
O1—C1	1.236 (8)	C4—H4A	0.9300
O2—C1	1.258 (9)	C5—H5A	0.9300
N1—N2	1.229 (8)		
N1—Cu1—N4	97.9 (3)	Cu1—N1—N2	115.2 (5)
N1—Cu1—N4 ⁱ	101.4 (2)	Cu2—N1—N2	115.3 (5)
O2 ⁱⁱ —Cu1—N1	91.3 (2)	N1—N2—N3	178.9 (8)
N1—Cu1—N7 ⁱⁱ	155.5 (2)	Cu1—N4—N5	122.8 (5)

N4—Cu1—N4 ⁱ	85.8 (2)	Cu1—N4—Cu1 ⁱ	94.2 (2)
O2 ⁱⁱ —Cu1—N4	167.4 (2)	Cu1 ⁱ —N4—N5	99.0 (4)
N4—Cu1—N7 ⁱⁱ	93.4 (3)	N4—N5—N6	175.6 (7)
O2 ⁱⁱ —Cu1—N4 ⁱ	83.89 (19)	C2—N7—C5	117.2 (6)
N4 ⁱ —Cu1—N7 ⁱⁱ	101.0 (2)	Cu1 ⁱⁱ —N7—C2	112.0 (4)
O2 ⁱⁱ —Cu1—N7 ⁱⁱ	81.5 (2)	Cu1 ⁱⁱ —N7—C5	130.6 (5)
O1—Cu2—N1	88.1 (2)	Cu2—N8—C2	114.5 (4)
O1—Cu2—N8	79.4 (2)	Cu2—N8—C3	127.6 (6)
O1—Cu2—O1 ⁱⁱⁱ	180.00	C2—N8—C3	117.8 (6)
O1—Cu2—N1 ⁱⁱⁱ	91.9 (2)	O1—C1—O2	127.6 (6)
O1—Cu2—N8 ⁱⁱⁱ	100.6 (2)	O1—C1—C2	117.9 (6)
N1—Cu2—N8	90.8 (2)	O2—C1—C2	114.4 (6)
O1 ⁱⁱⁱ —Cu2—N1	91.9 (2)	N7—C2—N8	125.6 (6)
N1—Cu2—N1 ⁱⁱⁱ	180.00	N7—C2—C1	115.3 (6)
N1—Cu2—N8 ⁱⁱⁱ	89.2 (2)	N8—C2—C1	119.1 (6)
O1 ⁱⁱⁱ —Cu2—N8	100.6 (2)	N8—C3—C4	120.4 (8)
N1 ⁱⁱⁱ —Cu2—N8	89.2 (2)	C3—C4—C5	117.9 (7)
N8—Cu2—N8 ⁱⁱⁱ	180.00	N7—C5—C4	121.1 (7)
O1 ⁱⁱⁱ —Cu2—N1 ⁱⁱⁱ	88.1 (2)	N8—C3—H3A	120.00
O1 ⁱⁱⁱ —Cu2—N8 ⁱⁱⁱ	79.4 (2)	C4—C3—H3A	120.00
N1 ⁱⁱⁱ —Cu2—N8 ⁱⁱⁱ	90.8 (2)	C3—C4—H4A	121.00
Cu2—O1—C1	109.0 (4)	C5—C4—H4A	121.00
Cu1 ⁱⁱ —O2—C1	116.6 (4)	N7—C5—H5A	119.00
Cu1—N1—Cu2	116.8 (3)	C4—C5—H5A	119.00
O1—Cu1—N1—N2	136.0 (5)	N8—Cu2—N1—Cu1	84.3 (3)
N4—Cu1—N1—Cu2	103.7 (3)	N8—Cu2—N1—N2	-55.7 (6)
N4—Cu1—N1—N2	-116.3 (5)	O1 ⁱⁱⁱ —Cu2—N1—Cu1	-175.1 (3)
N4 ⁱ —Cu1—N1—Cu2	-169.0 (3)	O1 ⁱⁱⁱ —Cu2—N1—N2	44.9 (6)
N4 ⁱ —Cu1—N1—N2	-28.9 (5)	N8 ⁱⁱⁱ —Cu2—N1—Cu1	-95.7 (3)
O2 ⁱⁱ —Cu1—N1—Cu2	-84.9 (3)	N8 ⁱⁱⁱ —Cu2—N1—N2	124.3 (6)
O2 ⁱⁱ —Cu1—N1—N2	55.1 (5)	O1—Cu2—N8—C2	-2.2 (4)
N7 ⁱⁱ —Cu1—N1—Cu2	-12.9 (8)	O1—Cu2—N8—C3	175.8 (6)
N7 ⁱⁱ —Cu1—N1—N2	127.2 (6)	N1—Cu2—N8—C2	-90.1 (5)
O1—Cu1—N4—N5	72.4 (6)	N1—Cu2—N8—C3	87.9 (6)
O1—Cu1—N4—Cu1 ⁱ	175.86 (15)	O1 ⁱⁱⁱ —Cu2—N8—C2	177.8 (4)
N1—Cu1—N4—N5	-2.6 (6)	O1 ⁱⁱⁱ —Cu2—N8—C3	-4.3 (6)
N1—Cu1—N4—Cu1 ⁱ	100.9 (2)	N1 ⁱⁱⁱ —Cu2—N8—C2	89.9 (5)
N4 ⁱ —Cu1—N4—N5	-103.5 (6)	N1 ⁱⁱⁱ —Cu2—N8—C3	-92.2 (6)
N4 ⁱ —Cu1—N4—Cu1 ⁱ	0.0 (2)	Cu1—O1—C1—O2	-91.6 (6)
N7 ⁱⁱ —Cu1—N4—N5	155.7 (6)	Cu1—O1—C1—C2	84.7 (5)
N7 ⁱⁱ —Cu1—N4—Cu1 ⁱ	-100.8 (2)	Cu2—O1—C1—O2	-175.2 (5)
N1—Cu1—N4 ⁱ —Cu1 ⁱ	-97.2 (3)	Cu2—O1—C1—C2	1.2 (6)

supplementary materials

N1—Cu1—N4 ⁱ —N5 ⁱ	138.6 (4)	Cu1 ⁱⁱ —O2—C1—O1	-178.1 (5)
N4—Cu1—N4 ⁱ —Cu1 ⁱ	0.0 (3)	Cu1 ⁱⁱ —O2—C1—C2	5.5 (6)
N4—Cu1—N4 ⁱ —N5 ⁱ	-124.2 (5)	C5—N7—C2—N8	-1.4 (9)
O1—Cu1—O2 ⁱⁱ —C1 ⁱⁱ	87.9 (4)	C5—N7—C2—C1	175.8 (5)
N1—Cu1—O2 ⁱⁱ —C1 ⁱⁱ	160.8 (4)	Cu1 ⁱⁱ —N7—C2—N8	-176.8 (5)
O1—Cu1—N7 ⁱⁱ —C2 ⁱⁱ	-84.5 (4)	Cu1 ⁱⁱ —N7—C2—C1	0.4 (6)
O1—Cu1—N7 ⁱⁱ —C5 ⁱⁱ	90.1 (6)	C2—N7—C5—C4	0.0 (10)
N1—Cu1—N7 ⁱⁱ —C2 ⁱⁱ	-75.9 (7)	Cu1 ⁱⁱ —N7—C5—C4	174.4 (5)
N1—Cu1—N7 ⁱⁱ —C5 ⁱⁱ	98.7 (7)	Cu2—N8—C2—N7	-179.3 (5)
N4—Cu1—N7 ⁱⁱ —C2 ⁱⁱ	166.6 (4)	Cu2—N8—C2—C1	3.6 (7)
N4—Cu1—N7 ⁱⁱ —C5 ⁱⁱ	-18.8 (6)	C3—N8—C2—N7	2.6 (9)
N1—Cu2—O1—Cu1	-2.98 (18)	C3—N8—C2—C1	-174.6 (6)
N1—Cu2—O1—C1	91.6 (4)	Cu2—N8—C3—C4	179.9 (5)
N8—Cu2—O1—Cu1	-94.14 (17)	C2—N8—C3—C4	-2.2 (10)
N8—Cu2—O1—C1	0.4 (4)	O1—C1—C2—N7	179.3 (5)
N1 ⁱⁱⁱ —Cu2—O1—Cu1	177.02 (18)	O1—C1—C2—N8	-3.3 (8)
N1 ⁱⁱⁱ —Cu2—O1—C1	-88.4 (4)	O2—C1—C2—N7	-3.9 (8)
N8 ⁱⁱⁱ —Cu2—O1—Cu1	85.86 (17)	O2—C1—C2—N8	173.5 (5)
N8 ⁱⁱⁱ —Cu2—O1—C1	-179.6 (4)	N8—C3—C4—C5	1.0 (11)
O1—Cu2—N1—Cu1	4.9 (3)	C3—C4—C5—N7	0.2 (11)
O1—Cu2—N1—N2	-135.1 (6)		

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

Fig. 1

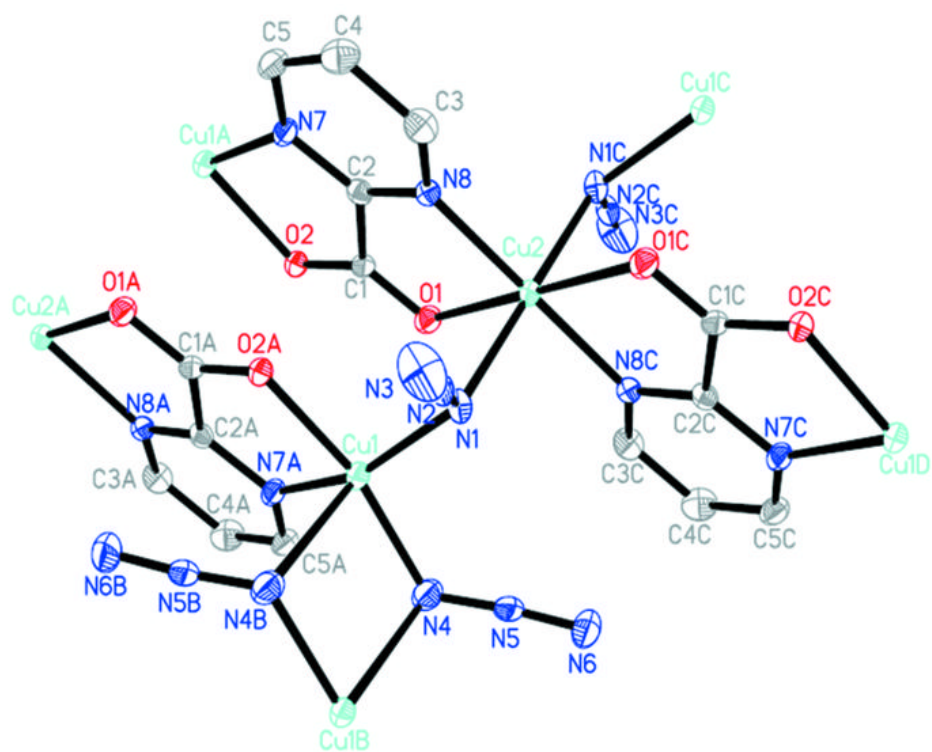


Fig. 2

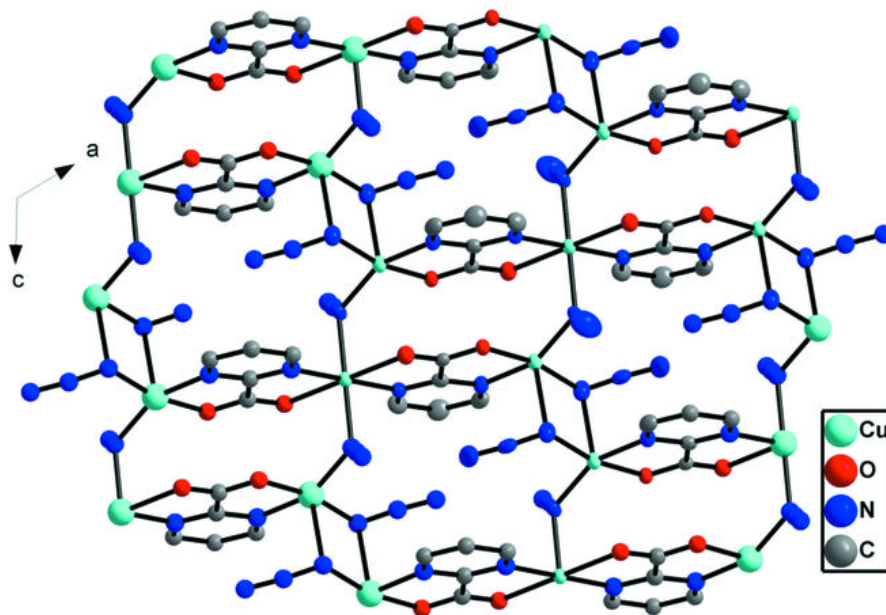


Fig. 3

