

Tetra- μ -acetato- κ^8 O:O'-bis{[4-methyl-N-(4-methylphenyl)pyridin-2-amine- κ N¹]-copper(II)}

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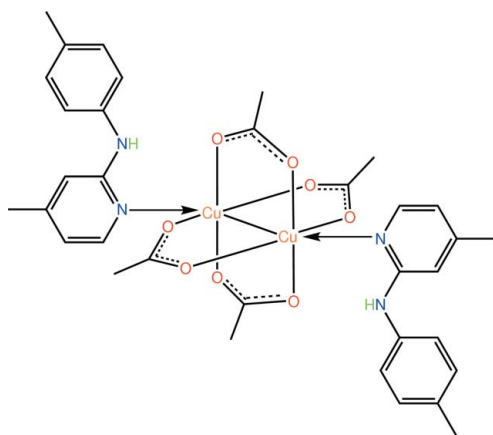
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.027; wR factor = 0.083; data-to-parameter ratio = 17.3.

The title complex, $[\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{C}_{13}\text{H}_{14}\text{N}_2)_2]$, features a binuclear molecule, which lies about a crystallographic centre of inversion; the four acetate ions each bridge a pair of Cu^{II} atoms. The coordination of the metal atom is distorted octahedral within a donor set defined by four O atoms, the heterocyclic N atom and the second Cu atom. The pyridine ring is twisted with respect to the tolyl ring and forms a dihedral angle of 35.34 (9)°. A bifurcated $\text{N}-\text{H}\cdots(\text{O},\text{O})$ hydrogen bond is present, linking the amine group to two carboxylate O atoms derived from different acetate ions. In the crystal, $\text{C}-\text{H}\cdots\pi$ interactions link molecules into a supramolecular array in the bc plane.

Related literature

For examples of tetrakisacetatobis[(substituted 2-amino-pyridyl)copper(II)] complexes, see: Barquín *et al.* (2004); Seco *et al.* (2004); Sieroń (2004); Fairuz *et al.* (2010).



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Experimental

Crystal data

$[\text{Cu}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{13}\text{H}_{14}\text{N}_2)_2]$
 $M_r = 759.78$
Monoclinic, $P2_1/c$
 $a = 11.7519$ (6) Å
 $b = 15.5822$ (8) Å
 $c = 9.9050$ (5) Å
 $\beta = 110.5698$ (6)°

$V = 1698.17$ (15) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.31$ mm⁻¹
 $T = 293$ K
 $0.40 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.648$, $T_{\text{max}} = 0.746$

16009 measured reflections
3890 independent reflections
3462 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.083$
 $S = 1.01$
3890 reflections
225 parameters
1 restraint

H atoms treated by a mixture of
independent and constrained
refinement

$\Delta\rho_{\text{max}} = 0.32$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—O2 ⁱ	1.9701 (13)	Cu1—O1	1.9759 (13)
Cu1—O3	1.9702 (14)	Cu1—N1	2.2016 (14)
Cu1—O4 ⁱ	1.9713 (14)	Cu1—Cu1 ⁱ	2.6480 (4)

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

Table 2

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the N1,C5–C9 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H2n ^{..} ·O1	0.85 (3)	2.36 (2)	3.117 (3)	149 (2)
N2—H2n ^{..} ·O4 ⁱ	0.85 (3)	2.46 (3)	3.047 (2)	127 (2)
C2—H2a ^{..} ·Cg1 ⁱⁱ	0.96	2.80	3.566 (2)	138

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5591).

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supplementary materials

Acta Cryst. (2010). E66, m1077-m1078 [doi:10.1107/S1600536810031168]

Tetra- μ -acetato- κ^8 O:O'-bis{[4-methyl-N-(4-methylphenyl)pyridin-2-amine- κ N¹]copper(II)}

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Comment

In connection with on-going studies into the structural characterization of tetrakisacetatobis[(substituted 2-aminopyridyl)copper] complexes, see: Barquín *et al.*, 2004; Seco *et al.*, 2004; Sieroń, 2004; Fairuz *et al.*, 2010), the binuclear title complex, (I), was investigated.

The binuclear copper(II) complex, Fig. 1, is situated about a centre of inversion and features two Cu^{II} atoms bridged by four acetate groups. The Cu–O bond distances lie in a narrow range, *i.e.* 1.9701 (13) to 1.9759 (13) Å, Table 1. The distorted octahedral coordination environment for the Cu atom is completed by a pyridine-N atom derived from the 4-methyl-*N-p*-tolylpyridin-2-amine ligand and the second Cu atom [Cuⁱ–Cuⁱ = 2.6480 (4) Å for *i*: 1 - *x*, 1 - *y*, 1 - *z*]. Two intramolecular N1–H \cdots O interactions are noted in which the amine-H spans carboxylate-O atoms derived from different ligands, Table 2. The dihedral angle formed between the pyridine and benzene rings of 35.34 (9) ° indicates the *N*-heterocycle is non-planar. The major twist in the molecule occurs around the amine group as seen in the value of the C9–N2–C11–C12 torsion angle of -27.2 (3) °. In the crystal packing, contacts of the type C–H \cdots π occur between methyl-H and pyridine rings, Table 2, and lead to the formation of supramolecular arrays in the *bc* plane, Fig. 2. Layers thus formed stack along the *a* axis, Fig. 3.

Experimental

Copper acetate (0.1 g, 0.5 mmol) dissolved in acetonitrile (15 ml) was added to a mixture of 4-methyl-*N-p*-tolylpyridin-2-amine (0.2183 g, 1.1 mmol) and trimethyl orthoformate (10 ml). The mixture was heated at 323 K, the green precipitate was collected and recrystallization from its acetonitrile solution yielded green prisms of (I).

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 to 0.96 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to 1.2 to 1.5 $U_{\text{equiv}}(\text{C})$. The N-bound H-atom was located in a difference Fourier map, and was refined with a distance restraint of N–H 0.86±0.01 Å; the U_{iso} value was freely refined

Figures

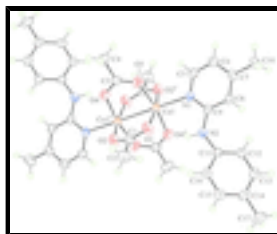


Fig. 1. The molecular structure of (I) showing displacement ellipsoids at the 50% probability level. Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*.

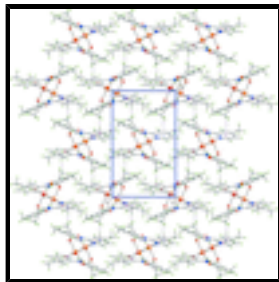


Fig. 2. Supramolecular arrays in the bc plane in (I) mediated by C–H \cdots π interactions shown as purple dashed lines.

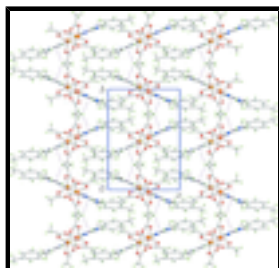


Fig. 3. Unit-cell contents shown in projection down the c axis in (I) showing the stacking of layers along a . The C–H \cdots π contacts are shown as purple dashed lines.

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Crystal data

[Cu₂(C₂H₃O₂)₄(C₁₃H₁₄N₂)₂]

$M_r = 759.78$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.7519$ (6) Å

$b = 15.5822$ (8) Å

$c = 9.9050$ (5) Å

$\beta = 110.5698$ (6)°

$V = 1698.17$ (15) Å³

$Z = 2$

$F(000) = 788$

$D_x = 1.486$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8249 reflections

$\theta = 4.3$ – 28.2 °

$\mu = 1.31$ mm⁻¹

$T = 293$ K

Prism, green

$0.40 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scan

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.648$, $T_{\max} = 0.746$

16009 measured reflections

3890 independent reflections

3462 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 1.9$ °

$h = -14 \rightarrow 15$

$k = -20 \rightarrow 19$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct
methods

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.027$$

$$wR(F^2) = 0.083$$

$$S = 1.01$$

3890 reflections

225 parameters

1 restraint

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.7683P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.566326 (17)	0.523188 (13)	0.42225 (2)	0.02759 (8)
N1	0.67899 (13)	0.56104 (9)	0.29545 (15)	0.0288 (3)
N2	0.83831 (15)	0.60834 (13)	0.48943 (17)	0.0431 (4)
H2n	0.7883 (19)	0.6036 (17)	0.533 (3)	0.060 (8)*
O1	0.59163 (14)	0.62952 (9)	0.53779 (16)	0.0456 (3)
O2	0.47897 (13)	0.59061 (9)	0.66720 (15)	0.0416 (3)
O3	0.41276 (12)	0.56868 (10)	0.28515 (15)	0.0449 (3)
O4	0.30200 (12)	0.52953 (10)	0.41638 (16)	0.0444 (3)
C1	0.54512 (15)	0.64284 (11)	0.63233 (19)	0.0319 (4)
C2	0.5712 (2)	0.72788 (14)	0.7088 (3)	0.0476 (5)
H2A	0.6411	0.7535	0.6962	0.071*
H2B	0.5870	0.7194	0.8098	0.071*
H2C	0.5023	0.7651	0.6694	0.071*
C3	0.31446 (16)	0.56196 (12)	0.30683 (19)	0.0343 (4)
C4	0.2011 (2)	0.59515 (18)	0.1922 (3)	0.0570 (6)
H4A	0.1309	0.5714	0.2067	0.086*
H4B	0.2013	0.5786	0.0989	0.086*
H4C	0.1989	0.6566	0.1979	0.086*
C5	0.62691 (17)	0.54835 (13)	0.1533 (2)	0.0376 (4)
H5	0.5491	0.5250	0.1193	0.045*
C6	0.68042 (18)	0.56738 (15)	0.0545 (2)	0.0426 (5)
H6	0.6405	0.5564	-0.0431	0.051*

supplementary materials

C7	0.79636 (18)	0.60370 (13)	0.1037 (2)	0.0381 (4)
C8	0.85144 (16)	0.61737 (12)	0.24918 (19)	0.0342 (4)
H8	0.9286	0.6417	0.2848	0.041*
C9	0.79178 (15)	0.59485 (11)	0.34396 (18)	0.0287 (3)
C10	0.8574 (2)	0.6289 (2)	−0.0006 (2)	0.0594 (7)
H10A	0.9330	0.5986	0.0225	0.089*
H10B	0.8725	0.6895	0.0059	0.089*
H10C	0.8056	0.6146	−0.0969	0.089*
C11	0.95658 (16)	0.62975 (12)	0.58042 (17)	0.0313 (4)
C12	1.06199 (17)	0.60942 (12)	0.5541 (2)	0.0351 (4)
H12	1.0573	0.5808	0.4700	0.042*
C13	1.17443 (17)	0.63203 (13)	0.6539 (2)	0.0383 (4)
H13	1.2441	0.6197	0.6335	0.046*
C14	1.18612 (17)	0.67236 (13)	0.7825 (2)	0.0391 (4)
C15	1.07993 (18)	0.69041 (14)	0.8091 (2)	0.0422 (4)
H15	1.0848	0.7165	0.8954	0.051*
C16	0.96734 (17)	0.67014 (14)	0.7092 (2)	0.0382 (4)
H16	0.8976	0.6838	0.7286	0.046*
C17	1.3088 (2)	0.69482 (19)	0.8908 (3)	0.0605 (6)
H17A	1.3591	0.7183	0.8416	0.091*
H17B	1.3464	0.6441	0.9423	0.091*
H17C	1.2993	0.7364	0.9575	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02400 (12)	0.03200 (13)	0.02806 (12)	−0.00382 (8)	0.01077 (8)	−0.00001 (7)
N1	0.0256 (7)	0.0335 (7)	0.0283 (7)	−0.0050 (6)	0.0107 (5)	−0.0009 (6)
N2	0.0290 (8)	0.0746 (12)	0.0281 (7)	−0.0196 (8)	0.0129 (6)	−0.0065 (7)
O1	0.0547 (9)	0.0384 (7)	0.0547 (8)	−0.0154 (6)	0.0331 (7)	−0.0131 (6)
O2	0.0451 (8)	0.0390 (7)	0.0475 (8)	−0.0118 (6)	0.0248 (6)	−0.0106 (6)
O3	0.0342 (7)	0.0612 (9)	0.0396 (7)	0.0082 (7)	0.0133 (6)	0.0156 (7)
O4	0.0285 (7)	0.0626 (10)	0.0407 (7)	0.0018 (6)	0.0102 (6)	0.0122 (6)
C1	0.0273 (8)	0.0305 (8)	0.0353 (9)	−0.0009 (7)	0.0076 (7)	−0.0028 (7)
C2	0.0500 (12)	0.0361 (10)	0.0557 (12)	−0.0078 (9)	0.0172 (10)	−0.0128 (9)
C3	0.0299 (9)	0.0369 (9)	0.0320 (8)	0.0046 (7)	0.0057 (7)	0.0001 (7)
C4	0.0399 (11)	0.0736 (16)	0.0467 (12)	0.0173 (11)	0.0017 (9)	0.0116 (11)
C5	0.0312 (9)	0.0492 (10)	0.0314 (9)	−0.0133 (8)	0.0097 (7)	−0.0049 (8)
C6	0.0404 (10)	0.0600 (13)	0.0270 (8)	−0.0120 (9)	0.0114 (7)	−0.0047 (8)
C7	0.0368 (9)	0.0497 (11)	0.0326 (9)	−0.0042 (8)	0.0183 (8)	0.0027 (8)
C8	0.0265 (8)	0.0438 (10)	0.0334 (8)	−0.0072 (7)	0.0120 (7)	0.0038 (7)
C9	0.0261 (8)	0.0316 (8)	0.0291 (8)	−0.0032 (6)	0.0107 (6)	−0.0002 (6)
C10	0.0529 (13)	0.0952 (19)	0.0381 (11)	−0.0155 (13)	0.0260 (10)	0.0041 (12)
C11	0.0277 (8)	0.0370 (9)	0.0283 (8)	−0.0073 (7)	0.0086 (6)	0.0016 (6)
C12	0.0355 (9)	0.0372 (9)	0.0335 (9)	−0.0017 (7)	0.0133 (7)	−0.0034 (7)
C13	0.0276 (8)	0.0427 (10)	0.0445 (10)	0.0012 (8)	0.0125 (8)	0.0025 (8)
C14	0.0301 (9)	0.0421 (10)	0.0386 (9)	−0.0039 (8)	0.0041 (7)	0.0025 (8)
C15	0.0406 (10)	0.0513 (11)	0.0316 (9)	−0.0028 (9)	0.0090 (8)	−0.0080 (8)

C16	0.0299 (9)	0.0535 (11)	0.0333 (9)	-0.0021 (8)	0.0135 (7)	-0.0029 (8)
C17	0.0357 (11)	0.0785 (17)	0.0535 (13)	-0.0105 (11)	-0.0015 (10)	-0.0050 (12)

Geometric parameters (Å, °)

Cu1—O2 ⁱ	1.9701 (13)	C5—C6	1.368 (3)
Cu1—O3	1.9702 (14)	C5—H5	0.9300
Cu1—O4 ⁱ	1.9713 (14)	C6—C7	1.396 (3)
Cu1—O1	1.9759 (13)	C6—H6	0.9300
Cu1—N1	2.2016 (14)	C7—C8	1.373 (3)
Cu1—Cu1 ⁱ	2.6480 (4)	C7—C10	1.502 (3)
N1—C5	1.339 (2)	C8—C9	1.400 (2)
N1—C9	1.348 (2)	C8—H8	0.9300
N2—C9	1.366 (2)	C10—H10A	0.9600
N2—C11	1.405 (2)	C10—H10B	0.9600
N2—H2n	0.85 (3)	C10—H10C	0.9600
O1—C1	1.256 (2)	C11—C16	1.388 (2)
O2—C1	1.255 (2)	C11—C12	1.389 (3)
O2—Cu1 ⁱ	1.9701 (13)	C12—C13	1.389 (3)
O3—C3	1.251 (2)	C12—H12	0.9300
O4—C3	1.251 (2)	C13—C14	1.384 (3)
O4—Cu1 ⁱ	1.9713 (14)	C13—H13	0.9300
C1—C2	1.504 (3)	C14—C15	1.391 (3)
C2—H2A	0.9600	C14—C17	1.505 (3)
C2—H2B	0.9600	C15—C16	1.382 (3)
C2—H2C	0.9600	C15—H15	0.9300
C3—C4	1.506 (3)	C16—H16	0.9300
C4—H4A	0.9600	C17—H17A	0.9600
C4—H4B	0.9600	C17—H17B	0.9600
C4—H4C	0.9600	C17—H17C	0.9600
O2 ⁱ —Cu1—O3	88.66 (7)	N1—C5—H5	117.8
O2 ⁱ —Cu1—O4 ⁱ	90.04 (7)	C6—C5—H5	117.8
O3—Cu1—O4 ⁱ	167.64 (6)	C5—C6—C7	118.40 (17)
O2 ⁱ —Cu1—O1	167.72 (6)	C5—C6—H6	120.8
O3—Cu1—O1	90.72 (7)	C7—C6—H6	120.8
O4 ⁱ —Cu1—O1	87.95 (7)	C8—C7—C6	118.17 (16)
O2 ⁱ —Cu1—N1	96.10 (5)	C8—C7—C10	121.22 (18)
O3—Cu1—N1	95.70 (5)	C6—C7—C10	120.60 (18)
O4 ⁱ —Cu1—N1	96.67 (6)	C7—C8—C9	120.16 (16)
O1—Cu1—N1	96.17 (5)	C7—C8—H8	119.9
O2 ⁱ —Cu1—Cu1 ⁱ	83.96 (4)	C9—C8—H8	119.9
O3—Cu1—Cu1 ⁱ	85.14 (4)	N1—C9—N2	114.53 (14)
O4 ⁱ —Cu1—Cu1 ⁱ	82.50 (4)	N1—C9—C8	121.36 (15)
O1—Cu1—Cu1 ⁱ	83.77 (4)	N2—C9—C8	124.04 (16)
N1—Cu1—Cu1 ⁱ	179.17 (4)	C7—C10—H10A	109.5

supplementary materials

C5—N1—C9	117.49 (14)	C7—C10—H10B	109.5
C5—N1—Cu1	114.60 (11)	H10A—C10—H10B	109.5
C9—N1—Cu1	127.91 (11)	C7—C10—H10C	109.5
C9—N2—C11	130.71 (15)	H10A—C10—H10C	109.5
C9—N2—H2n	115.7 (18)	H10B—C10—H10C	109.5
C11—N2—H2n	113.6 (18)	C16—C11—C12	118.46 (16)
C1—O1—Cu1	123.64 (12)	C16—C11—N2	116.57 (16)
C1—O2—Cu1 ⁱ	123.75 (12)	C12—C11—N2	124.87 (16)
C3—O3—Cu1	121.93 (12)	C13—C12—C11	119.80 (17)
C3—O4—Cu1 ⁱ	125.01 (12)	C13—C12—H12	120.1
O1—C1—O2	124.88 (16)	C11—C12—H12	120.1
O1—C1—C2	117.13 (17)	C12—C13—C14	122.15 (18)
O2—C1—C2	117.99 (17)	C12—C13—H13	118.9
C1—C2—H2A	109.5	C14—C13—H13	118.9
C1—C2—H2B	109.5	C13—C14—C15	117.41 (17)
H2A—C2—H2B	109.5	C13—C14—C17	121.47 (19)
C1—C2—H2C	109.5	C15—C14—C17	121.1 (2)
H2A—C2—H2C	109.5	C16—C15—C14	121.02 (18)
H2B—C2—H2C	109.5	C16—C15—H15	119.5
O4—C3—O3	125.38 (17)	C14—C15—H15	119.5
O4—C3—C4	116.79 (18)	C15—C16—C11	121.12 (18)
O3—C3—C4	117.83 (18)	C15—C16—H16	119.4
C3—C4—H4A	109.5	C11—C16—H16	119.4
C3—C4—H4B	109.5	C14—C17—H17A	109.5
H4A—C4—H4B	109.5	C14—C17—H17B	109.5
C3—C4—H4C	109.5	H17A—C17—H17B	109.5
H4A—C4—H4C	109.5	C14—C17—H17C	109.5
H4B—C4—H4C	109.5	H17A—C17—H17C	109.5
N1—C5—C6	124.41 (17)	H17B—C17—H17C	109.5
O2 ⁱ —Cu1—N1—C5	48.27 (14)	C9—N1—C5—C6	0.0 (3)
O3—Cu1—N1—C5	-40.99 (15)	Cu1—N1—C5—C6	179.90 (18)
O4 ⁱ —Cu1—N1—C5	139.02 (14)	N1—C5—C6—C7	-1.0 (3)
O1—Cu1—N1—C5	-132.33 (14)	C5—C6—C7—C8	0.9 (3)
Cu1 ⁱ —Cu1—N1—C5	142 (3)	C5—C6—C7—C10	-177.7 (2)
O2 ⁱ —Cu1—N1—C9	-131.83 (15)	C6—C7—C8—C9	0.2 (3)
O3—Cu1—N1—C9	138.92 (15)	C10—C7—C8—C9	178.8 (2)
O4 ⁱ —Cu1—N1—C9	-41.07 (15)	C5—N1—C9—N2	178.27 (18)
O1—Cu1—N1—C9	47.58 (15)	Cu1—N1—C9—N2	-1.6 (2)
Cu1 ⁱ —Cu1—N1—C9	-38 (3)	C5—N1—C9—C8	1.2 (3)
O2 ⁱ —Cu1—O1—C1	-2.9 (4)	Cu1—N1—C9—C8	-178.74 (13)
O3—Cu1—O1—C1	84.09 (16)	C11—N2—C9—N1	169.2 (2)
O4 ⁱ —Cu1—O1—C1	-83.62 (16)	C11—N2—C9—C8	-13.8 (3)
N1—Cu1—O1—C1	179.90 (16)	C7—C8—C9—N1	-1.3 (3)
Cu1 ⁱ —Cu1—O1—C1	-0.94 (15)	C7—C8—C9—N2	-178.1 (2)
O2 ⁱ —Cu1—O3—C3	82.85 (16)	C9—N2—C11—C16	156.4 (2)
O4 ⁱ —Cu1—O3—C3	-1.2 (4)	C9—N2—C11—C12	-27.2 (3)

O1—Cu1—O3—C3	-84.89 (16)	C16—C11—C12—C13	-2.0 (3)
N1—Cu1—O3—C3	178.84 (16)	N2—C11—C12—C13	-178.34 (18)
Cu1 ⁱ —Cu1—O3—C3	-1.20 (15)	C11—C12—C13—C14	2.0 (3)
Cu1—O1—C1—O2	1.2 (3)	C12—C13—C14—C15	-0.4 (3)
Cu1—O1—C1—C2	-178.81 (14)	C12—C13—C14—C17	178.7 (2)
Cu1 ⁱ —O2—C1—O1	-0.6 (3)	C13—C14—C15—C16	-1.2 (3)
Cu1 ⁱ —O2—C1—C2	179.40 (14)	C17—C14—C15—C16	179.7 (2)
Cu1 ⁱ —O4—C3—O3	-2.7 (3)	C14—C15—C16—C11	1.2 (3)
Cu1 ⁱ —O4—C3—C4	177.10 (15)	C12—C11—C16—C15	0.4 (3)
Cu1—O3—C3—O4	2.6 (3)	N2—C11—C16—C15	177.08 (19)
Cu1—O3—C3—C4	-177.18 (15)		

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

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N1,C5–C9 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2n \cdots O1	0.85 (3)	2.36 (2)	3.117 (3)	149 (2)
N2—H2n \cdots O4 ⁱ	0.85 (3)	2.46 (3)	3.047 (2)	127 (2)
C2—H2a \cdots Cg1 ⁱⁱ	0.96	2.80	3.566 (2)	138

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+3/2, z+1/2$.

Fig. 1

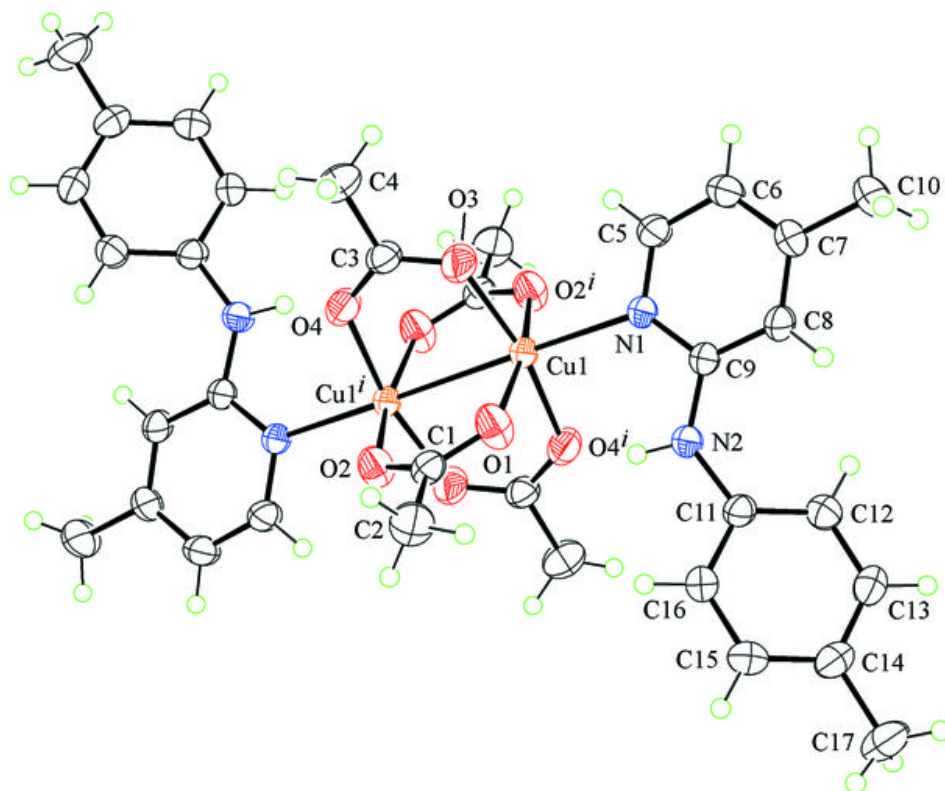


Fig. 2

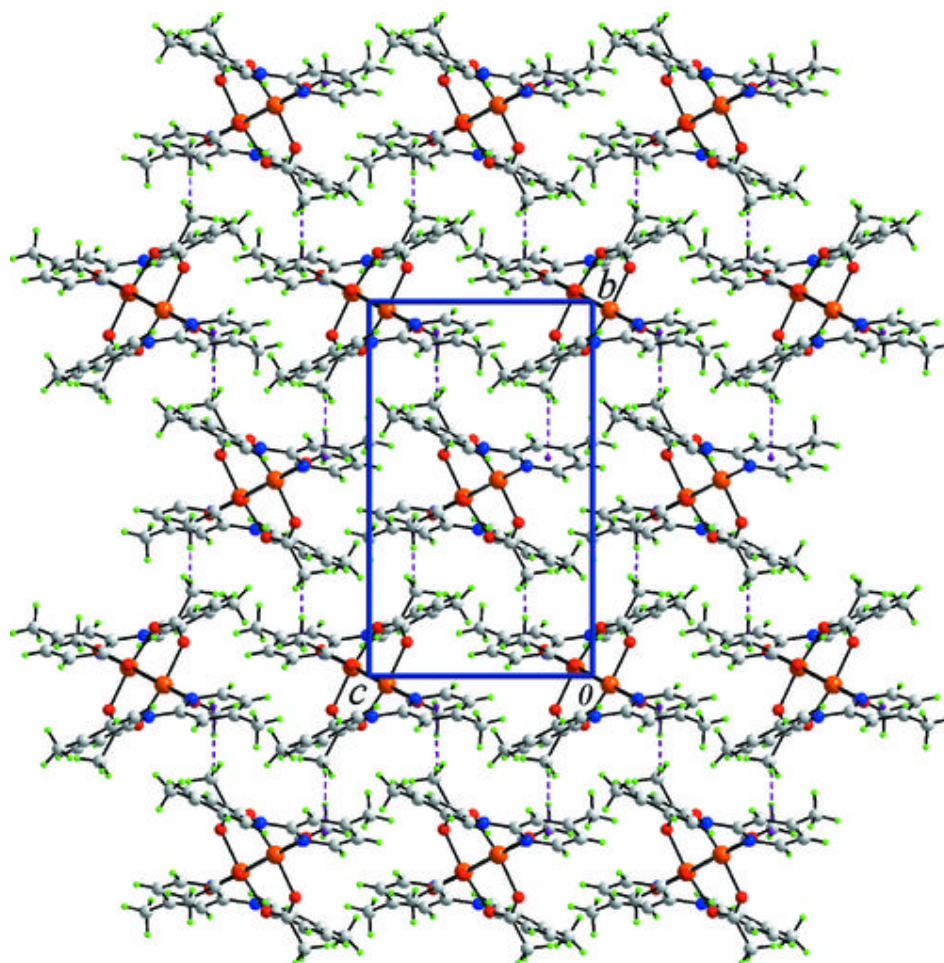


Fig. 3

