

Bis(μ -biphenyl-2,2'-dicarboxylato)-bis[(2,2'-bipyridine)copper(II)]

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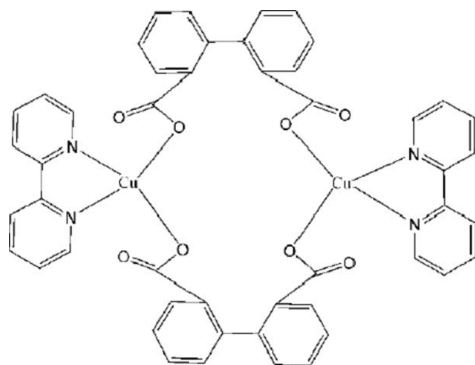
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.037; wR factor = 0.118; data-to-parameter ratio = 16.0.

The title compound, $[\text{Cu}_2(\text{C}_{14}\text{H}_8\text{O}_4)_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]$, is a centrosymmetric binuclear copper(II) complex, with a $\text{Cu}\cdots\text{Cu}$ separation of 6.136 (16) Å. The Cu atom displays a *cis*- CuN_2O_2 square-planar geometry, although two long (> 2.43 Å) $\text{Cu}\cdots\text{O}$ contacts complete a distorted *cis*- CuN_2O_4 octahedron. Extensive $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For related literature, see: Bu *et al.* (2004); He *et al.* (2007); Huang *et al.* (2004); Long *et al.* (2001); Ma *et al.* (2003); Rao *et al.* (2004); Yaghi *et al.* (2003); Yang *et al.* (2002); Zhang *et al.* (2004); Zhu *et al.* (2001); He & Zhu (2003).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_{14}\text{H}_8\text{O}_4)_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]$

$M_r = 1839.75$

Monoclinic, $P2_1/c$

$a = 11.234$ (2) Å

$b = 13.336$ (3) Å

$c = 15.431$ (6) Å

$\beta = 122.16$ (2)°

$V = 1957.1$ (9) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.15$ mm⁻¹

$T = 293$ (2) K

$0.40 \times 0.26 \times 0.23$ mm

Data collection

Siemens SMART CCD area-detector diffractometer

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

$T_{\min} = 0.708$, $T_{\max} = 0.771$

18687 measured reflections

4472 independent reflections

3708 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.118$

$S = 1.03$

4472 reflections

280 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.29$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9640 (15)	Cu1—N1	1.9897 (19)
Cu1—O4 ⁱ	1.9725 (16)	Cu1—O2	2.434 (2)
Cu1—N2	1.9814 (19)	Cu1—O3 ⁱ	2.557 (2)
O1—Cu1—O4 ⁱ	93.92 (7)	O1—Cu1—N1	94.56 (7)
O1—Cu1—N2	162.77 (7)	O4 ⁱ —Cu1—N1	160.15 (7)
O4 ⁱ —Cu1—N2	95.38 (8)	N2—Cu1—N1	81.35 (8)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1A \cdots O1	0.93	2.58	3.081 (3)	114
C4—H4A \cdots O4 ⁱⁱ	0.93	2.59	3.378 (3)	143
C5—H5A \cdots O4 ⁱⁱⁱ	0.93	2.51	3.304 (4)	144
C6—H6A \cdots O3 ⁱⁱⁱ	0.93	2.25	3.162 (3)	166
C16—H16A \cdots O2 ^{iv}	0.93	2.48	3.192 (3)	133
C19—H19A \cdots O4	0.93	2.45	2.761 (3)	100

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

Data collection: SMART (Siemens, 1994); cell refinement: SAINT (Siemens, 1994); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2255).

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supplementary materials

Acta Cryst. (2008). E64, m1171-m1172 [doi:10.1107/S160053680802583X]

Bis(μ -biphenyl-2,2'-dicarboxylato)bis[(2,2'-bipyridine)copper(II)]

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Comment

Design and assembly of metal-involved supramolecular architectures are currently of great interest in the field of supramolecular chemistry and crystal engineering because they can provide novel topology and functional materials (Yaghi *et al.*, 2003; Rao *et al.*, 2004). During the past decades, extensive efforts have been focused on the design and assembly of such kinds of supramolecular architectures (Huang *et al.*, 2004; Zhang *et al.*, 2004). By precisely selecting the modular building unit, chemists now have successfully synthesized a great variety of one-dimensional, two-dimensional, and three-dimensional supramolecular architectures (Bu *et al.*, 2004; Ma *et al.*, 2003; Yang *et al.*, 2002; Long *et al.*, 2001). Binuclear copper(II) complexes have been intensely investigated owing to their potential application as magnetic materials and catalysts (Zhu *et al.*, 2001). In this work, we employed H₂dpa (dpa = diphenyl-2,2'-dicarboxylato dianion) and 2,2'-bipyridine (bipy) ligands for producing a binuclear complex, [Cu₂(C₁₄H₈O₄)₂(C₁₀H₈N₂)₂].

The compound contains a centrosymmetric binuclear complex. The copper(II) atom in the title compound adopts a distorted square geometry (Table 1, Fig. 1). The bipy ligand shows its classical bidentate coordination mode, with a similar Cu—N bond length to that the related complex [Cu₂(C₁₄H₈O₄)₂(C₁₀H₈N₂)₂].4H₂O (He *et al.*, 2007). The dpa ligand adopts a μ -bridged coordination and the dihedral angle between its aromatic rings is 78.27°. As well as the short Cu—O bonds, two long Cu—O (Cu(1)—O(2): 2.434 (44) Å; Cu(1)—O(3): 2.557 (31) Å) contacts that might be regarded as secondary bonds (He & Zhu, 2003) complete a distorted octahedron. The Cu \cdots Cuⁱ (i = 1 - x, -y, -z) distance bridged by the dpa ligands is 6.136 (16) Å. Extensive C—H \cdots O hydrogen bonds link molecules into a three-dimensional network. (Table 2, Fig. 2).

Experimental

A solution of Cu(NO₃)₂·6H₂O (0.0705 g) in 5 ml of water was added dropwise under continuous stirring to an aqueous solution (5 ml) of diphenyl-2,2'-dicarboxylic acid (0.0734 g) and 2,2'-bipyridine (0.0312 g). The resulting mixture was then transferred into a 25 ml Teflon-lined stainless steel vessel, which was sealed and heated to 423 K for 72 h, then cooled to room temperature. The block blue single crystals were obtained.

Refinement

The phenyl H atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

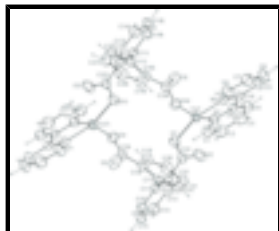


Fig. 1. View of the structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level; H-atoms are shown as small spheres of arbitrary radius.

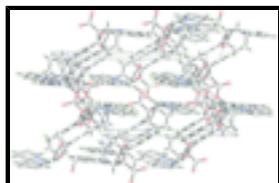


Fig. 2. View of the 3D hydrogen-bonded network in the packing of the title compound. The packing is viewed along the *b* axis; C—H...O interactions are shown as dashed lines.

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Crystal data

[Cu₂(C₁₄H₈O₄)₂(C₁₀H₈N₂)₂]

$M_r = 1839.75$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.234 (2) \text{ \AA}$

$b = 13.336 (3) \text{ \AA}$

$c = 15.431 (6) \text{ \AA}$

$\beta = 122.16 (2)^\circ$

$V = 1957.1 (9) \text{ \AA}^3$

$Z = 2$

$F_{000} = 940$

$D_x = 1.561 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 19150 reflections

$\theta = 3.1\text{--}27.4^\circ$

$\mu = 1.15 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Block, blue

$0.40 \times 0.26 \times 0.23 \text{ mm}$

Data collection

Siemens SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2) \text{ K}$

ω scans

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

$T_{\min} = 0.708$, $T_{\max} = 0.771$

18687 measured reflections

4472 independent reflections

3708 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 27.4^\circ$

$\theta_{\min} = 3.1^\circ$

$h = -14 \rightarrow 14$

$k = -17 \rightarrow 17$

$l = -18 \rightarrow 19$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.036$$

$$wR(F^2) = 0.118$$

$$S = 1.04$$

4472 reflections

280 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$$

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

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

$$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

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	0.63909 (3)	-0.160660 (19)	-0.059678 (18)	0.02914 (12)
O1	0.70349 (16)	-0.04363 (11)	0.03157 (11)	0.0354 (4)
O2	0.8638 (2)	-0.16096 (12)	0.10287 (15)	0.0530 (5)
O3	0.62962 (19)	0.15631 (14)	0.16045 (14)	0.0480 (5)
O4	0.47467 (16)	0.21452 (12)	0.00754 (11)	0.0374 (4)
N1	0.68794 (18)	-0.10223 (14)	-0.15551 (13)	0.0320 (4)
N2	0.63566 (18)	-0.28542 (14)	-0.13069 (14)	0.0331 (4)
C1	0.7186 (2)	-0.00573 (19)	-0.15928 (18)	0.0406 (5)
H1A	0.7227	0.0390	-0.1115	0.049*
C2	0.7441 (3)	0.0289 (2)	-0.2320 (2)	0.0504 (7)
H2A	0.7664	0.0959	-0.2327	0.060*
C3	0.7361 (3)	-0.0368 (2)	-0.3032 (2)	0.0531 (7)
H3A	0.7514	-0.0145	-0.3536	0.064*
C4	0.7051 (3)	-0.1367 (2)	-0.29961 (19)	0.0462 (6)
H4A	0.7002	-0.1823	-0.3470	0.055*
C5	0.6486 (3)	-0.3529 (2)	-0.2682 (2)	0.0487 (7)
H5A	0.6566	-0.3429	-0.3246	0.058*
C6	0.6319 (3)	-0.4472 (2)	-0.2420 (3)	0.0585 (8)
H6A	0.6296	-0.5022	-0.2800	0.070*
C7	0.6184 (3)	-0.4608 (2)	-0.1591 (2)	0.0540 (7)
H7A	0.6097	-0.5248	-0.1392	0.065*
C8	0.6181 (3)	-0.37789 (19)	-0.1068 (2)	0.0444 (6)

supplementary materials

H8A	0.6053	-0.3865	-0.0525	0.053*
C9	0.6815 (2)	-0.16746 (17)	-0.22479 (17)	0.0332 (5)
C10	0.6534 (2)	-0.27237 (17)	-0.20994 (17)	0.0337 (5)
C11	0.8922 (2)	0.08967 (16)	0.20040 (15)	0.0278 (4)
C12	0.8946 (2)	-0.01519 (16)	0.20175 (15)	0.0281 (4)
C13	0.9639 (2)	-0.06631 (17)	0.29523 (16)	0.0346 (5)
H13A	0.9681	-0.1360	0.2959	0.042*
C14	1.0260 (2)	-0.0142 (2)	0.38647 (16)	0.0405 (5)
H14A	1.0703	-0.0486	0.4484	0.049*
C15	1.0221 (2)	0.0895 (2)	0.38529 (17)	0.0419 (6)
H15A	1.0636	0.1249	0.4466	0.050*
C16	0.9568 (2)	0.14064 (17)	0.29350 (18)	0.0365 (5)
H16A	0.9559	0.2104	0.2937	0.044*
C17	0.8383 (2)	0.14901 (14)	0.10351 (17)	0.0282 (4)
C18	0.7102 (2)	0.19898 (15)	0.04996 (16)	0.0292 (4)
C19	0.6773 (2)	0.25507 (18)	-0.03716 (18)	0.0369 (5)
H19A	0.5920	0.2890	-0.0727	0.044*
C20	0.7682 (3)	0.26123 (18)	-0.07140 (19)	0.0412 (5)
H20A	0.7446	0.2991	-0.1290	0.049*
C21	0.8951 (2)	0.21017 (18)	-0.01881 (19)	0.0400 (5)
H21A	0.9573	0.2131	-0.0412	0.048*
C22	0.9287 (3)	0.15476 (17)	0.06719 (19)	0.0366 (5)
H22A	1.0137	0.1204	0.1018	0.044*
C23	0.8187 (2)	-0.07766 (15)	0.10614 (16)	0.0300 (4)
C24	0.5999 (2)	0.18908 (16)	0.07706 (17)	0.0309 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03431 (18)	0.02951 (18)	0.02666 (17)	-0.00125 (10)	0.01828 (13)	-0.00287 (9)
O1	0.0386 (8)	0.0330 (8)	0.0287 (8)	0.0015 (7)	0.0138 (7)	-0.0053 (6)
O2	0.0586 (12)	0.0359 (10)	0.0433 (10)	0.0155 (8)	0.0128 (9)	-0.0077 (7)
O3	0.0446 (10)	0.0630 (12)	0.0467 (11)	0.0160 (8)	0.0313 (9)	0.0260 (8)
O4	0.0328 (8)	0.0494 (10)	0.0328 (8)	0.0021 (7)	0.0193 (7)	0.0047 (7)
N1	0.0321 (9)	0.0371 (10)	0.0286 (9)	-0.0026 (8)	0.0174 (8)	-0.0026 (8)
N2	0.0323 (9)	0.0339 (10)	0.0325 (9)	0.0008 (8)	0.0168 (8)	-0.0031 (8)
C1	0.0441 (13)	0.0396 (13)	0.0410 (13)	-0.0049 (11)	0.0247 (11)	0.0004 (10)
C2	0.0523 (15)	0.0506 (16)	0.0521 (16)	-0.0115 (13)	0.0304 (13)	0.0044 (12)
C3	0.0485 (15)	0.075 (2)	0.0423 (14)	-0.0104 (14)	0.0288 (12)	0.0046 (13)
C4	0.0412 (13)	0.0684 (17)	0.0339 (12)	-0.0086 (12)	0.0233 (11)	-0.0095 (12)
C5	0.0477 (15)	0.0549 (17)	0.0515 (16)	-0.0021 (12)	0.0317 (13)	-0.0170 (12)
C6	0.0578 (17)	0.0476 (16)	0.074 (2)	-0.0064 (13)	0.0380 (16)	-0.0293 (15)
C7	0.0522 (16)	0.0322 (13)	0.076 (2)	-0.0053 (12)	0.0327 (15)	-0.0113 (12)
C8	0.0475 (14)	0.0354 (13)	0.0500 (15)	-0.0028 (11)	0.0259 (12)	-0.0028 (11)
C9	0.0253 (10)	0.0467 (13)	0.0273 (11)	-0.0003 (9)	0.0138 (9)	-0.0040 (9)
C10	0.0268 (10)	0.0414 (13)	0.0313 (11)	-0.0001 (9)	0.0144 (9)	-0.0076 (9)
C11	0.0261 (9)	0.0282 (10)	0.0298 (10)	0.0002 (8)	0.0154 (8)	-0.0003 (8)
C12	0.0282 (10)	0.0304 (11)	0.0269 (10)	0.0008 (8)	0.0154 (8)	0.0001 (8)

C13	0.0383 (12)	0.0330 (11)	0.0337 (11)	0.0039 (9)	0.0199 (10)	0.0056 (9)
C14	0.0416 (13)	0.0515 (14)	0.0261 (11)	0.0053 (11)	0.0166 (10)	0.0062 (10)
C15	0.0418 (12)	0.0521 (15)	0.0258 (11)	0.0020 (11)	0.0139 (10)	-0.0096 (10)
C16	0.0386 (12)	0.0322 (11)	0.0365 (12)	0.0003 (9)	0.0184 (10)	-0.0055 (9)
C17	0.0328 (11)	0.0243 (10)	0.0302 (11)	-0.0037 (8)	0.0186 (9)	-0.0015 (8)
C18	0.0345 (11)	0.0242 (10)	0.0320 (11)	-0.0024 (9)	0.0198 (9)	0.0004 (8)
C19	0.0403 (12)	0.0332 (12)	0.0382 (12)	0.0040 (10)	0.0215 (10)	0.0099 (10)
C20	0.0530 (14)	0.0362 (12)	0.0422 (13)	-0.0049 (11)	0.0305 (11)	0.0083 (10)
C21	0.0462 (13)	0.0398 (13)	0.0487 (14)	-0.0066 (11)	0.0352 (12)	0.0014 (11)
C22	0.0339 (12)	0.0389 (13)	0.0394 (13)	-0.0010 (9)	0.0211 (10)	0.0007 (9)
C23	0.0357 (11)	0.0280 (11)	0.0294 (10)	-0.0010 (9)	0.0194 (9)	-0.0010 (8)
C24	0.0346 (11)	0.0257 (10)	0.0360 (11)	0.0013 (9)	0.0211 (9)	0.0030 (9)

Geometric parameters (Å, °)

Cu1—O1	1.9640 (15)	C6—H6A	0.9300
Cu1—O4 ⁱ	1.9725 (16)	C7—C8	1.370 (4)
Cu1—N2	1.9814 (19)	C7—H7A	0.9300
Cu1—N1	1.9897 (19)	C8—H8A	0.9300
Cu1—O2	2.434 (2)	C9—C10	1.479 (3)
Cu1—C23	2.519 (2)	C11—C16	1.394 (3)
Cu1—O3 ⁱ	2.557 (2)	C11—C12	1.399 (3)
Cu1—C24 ⁱ	2.580 (2)	C11—C17	1.505 (3)
O1—C23	1.273 (2)	C12—C13	1.399 (3)
O2—C23	1.233 (3)	C12—C23	1.503 (3)
O3—C24	1.225 (3)	C13—C14	1.381 (3)
O3—Cu1 ⁱ	2.5567 (19)	C13—H13A	0.9300
O4—C24	1.280 (3)	C14—C15	1.383 (4)
O4—Cu1 ⁱ	1.9725 (16)	C14—H14A	0.9300
N1—C1	1.342 (3)	C15—C16	1.380 (3)
N1—C9	1.350 (3)	C15—H15A	0.9300
N2—C8	1.331 (3)	C16—H16A	0.9300
N2—C10	1.351 (3)	C17—C18	1.390 (3)
C1—C2	1.377 (3)	C17—C22	1.399 (3)
C1—H1A	0.9300	C18—C19	1.405 (3)
C2—C3	1.372 (4)	C18—C24	1.509 (3)
C2—H2A	0.9300	C19—C20	1.379 (3)
C3—C4	1.385 (4)	C19—H19A	0.9300
C3—H3A	0.9300	C20—C21	1.387 (3)
C4—C9	1.377 (3)	C20—H20A	0.9300
C4—H4A	0.9300	C21—C22	1.384 (3)
C5—C6	1.365 (4)	C21—H21A	0.9300
C5—C10	1.383 (3)	C22—H22A	0.9300
C5—H5A	0.9300	C24—Cu1 ⁱ	2.580 (2)
C6—C7	1.378 (5)		
O1—Cu1—O4 ⁱ	93.92 (7)	C6—C7—H7A	120.8
O1—Cu1—N2	162.77 (7)	N2—C8—C7	122.5 (3)

supplementary materials

O4 ⁱ —Cu1—N2	95.38 (8)	N2—C8—H8A	118.8
O1—Cu1—N1	94.56 (7)	C7—C8—H8A	118.8
O4 ⁱ —Cu1—N1	160.15 (7)	N1—C9—C4	121.3 (2)
N2—Cu1—N1	81.35 (8)	N1—C9—C10	114.4 (2)
O1—Cu1—O2	58.55 (6)	C4—C9—C10	124.3 (2)
O4 ⁱ —Cu1—O2	96.94 (8)	N2—C10—C5	121.0 (2)
N2—Cu1—O2	105.83 (7)	N2—C10—C9	114.12 (19)
N1—Cu1—O2	102.80 (8)	C5—C10—C9	124.9 (2)
O1—Cu1—C23	29.83 (6)	C16—C11—C12	118.49 (19)
O4 ⁱ —Cu1—C23	95.07 (7)	C16—C11—C17	118.75 (19)
N2—Cu1—C23	134.42 (7)	C12—C11—C17	122.34 (18)
N1—Cu1—C23	101.19 (7)	C11—C12—C13	119.90 (19)
O2—Cu1—C23	28.76 (6)	C11—C12—C23	122.91 (18)
O1—Cu1—O3 ⁱ	106.45 (7)	C13—C12—C23	117.11 (19)
O4 ⁱ —Cu1—O3 ⁱ	56.28 (6)	C14—C13—C12	120.5 (2)
N2—Cu1—O3 ⁱ	90.78 (7)	C14—C13—H13A	119.7
N1—Cu1—O3 ⁱ	104.04 (7)	C12—C13—H13A	119.7
O2—Cu1—O3 ⁱ	150.22 (7)	C13—C14—C15	119.7 (2)
C23—Cu1—O3 ⁱ	130.98 (7)	C13—C14—H14A	120.2
O1—Cu1—C24 ⁱ	99.04 (7)	C15—C14—H14A	120.2
O4 ⁱ —Cu1—C24 ⁱ	28.92 (6)	C16—C15—C14	120.2 (2)
N2—Cu1—C24 ⁱ	96.11 (7)	C16—C15—H15A	119.9
N1—Cu1—C24 ⁱ	131.58 (7)	C14—C15—H15A	119.9
O2—Cu1—C24 ⁱ	123.91 (8)	C15—C16—C11	121.2 (2)
C23—Cu1—C24 ⁱ	113.37 (7)	C15—C16—H16A	119.4
O3 ⁱ —Cu1—C24 ⁱ	27.59 (6)	C11—C16—H16A	119.4
C23—O1—Cu1	100.02 (13)	C18—C17—C22	118.57 (19)
C23—O2—Cu1	79.48 (13)	C18—C17—C11	125.76 (19)
C24—O3—Cu1 ⁱ	77.28 (13)	C22—C17—C11	115.66 (19)
C24—O4—Cu1 ⁱ	102.92 (13)	C17—C18—C19	119.05 (19)
C1—N1—C9	119.4 (2)	C17—C18—C24	122.42 (19)
C1—N1—Cu1	125.93 (16)	C19—C18—C24	118.37 (19)
C9—N1—Cu1	114.61 (15)	C20—C19—C18	121.8 (2)
C8—N2—C10	119.0 (2)	C20—C19—H19A	119.1
C8—N2—Cu1	125.93 (17)	C18—C19—H19A	119.1
C10—N2—Cu1	115.06 (15)	C19—C20—C21	119.1 (2)
N1—C1—C2	121.8 (2)	C19—C20—H20A	120.4
N1—C1—H1A	119.1	C21—C20—H20A	120.4
C2—C1—H1A	119.1	C22—C21—C20	119.6 (2)
C3—C2—C1	119.0 (3)	C22—C21—H21A	120.2
C3—C2—H2A	120.5	C20—C21—H21A	120.2
C1—C2—H2A	120.5	C21—C22—C17	121.9 (2)
C2—C3—C4	119.5 (2)	C21—C22—H22A	119.1
C2—C3—H3A	120.2	C17—C22—H22A	119.1
C4—C3—H3A	120.2	O2—C23—O1	121.8 (2)

C9—C4—C3	119.0 (2)	O2—C23—C12	120.6 (2)
C9—C4—H4A	120.5	O1—C23—C12	117.53 (18)
C3—C4—H4A	120.5	O2—C23—Cu1	71.76 (13)
C6—C5—C10	119.1 (3)	O1—C23—Cu1	50.14 (10)
C6—C5—H5A	120.4	C12—C23—Cu1	165.85 (15)
C10—C5—H5A	120.4	O3—C24—O4	122.5 (2)
C5—C6—C7	119.8 (2)	O3—C24—C18	121.2 (2)
C5—C6—H6A	120.1	O4—C24—C18	116.28 (18)
C7—C6—H6A	120.1	O3—C24—Cu1 ⁱ	75.13 (13)
C8—C7—C6	118.5 (3)	O4—C24—Cu1 ⁱ	48.16 (10)
C8—C7—H7A	120.8	C18—C24—Cu1 ⁱ	161.10 (15)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<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>
C1—H1A \cdots O1	0.93	2.58	3.081 (3)	114
C4—H4A \cdots O4 ⁱⁱ	0.93	2.59	3.378 (3)	143
C5—H5A \cdots O4 ⁱⁱ	0.93	2.51	3.304 (4)	144
C6—H6A \cdots O3 ⁱⁱⁱ	0.93	2.25	3.162 (3)	166
C16—H16A \cdots O2 ^{iv}	0.93	2.48	3.192 (3)	133
C19—H19A \cdots O4	0.93	2.45	2.761 (3)	100

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

Fig. 1

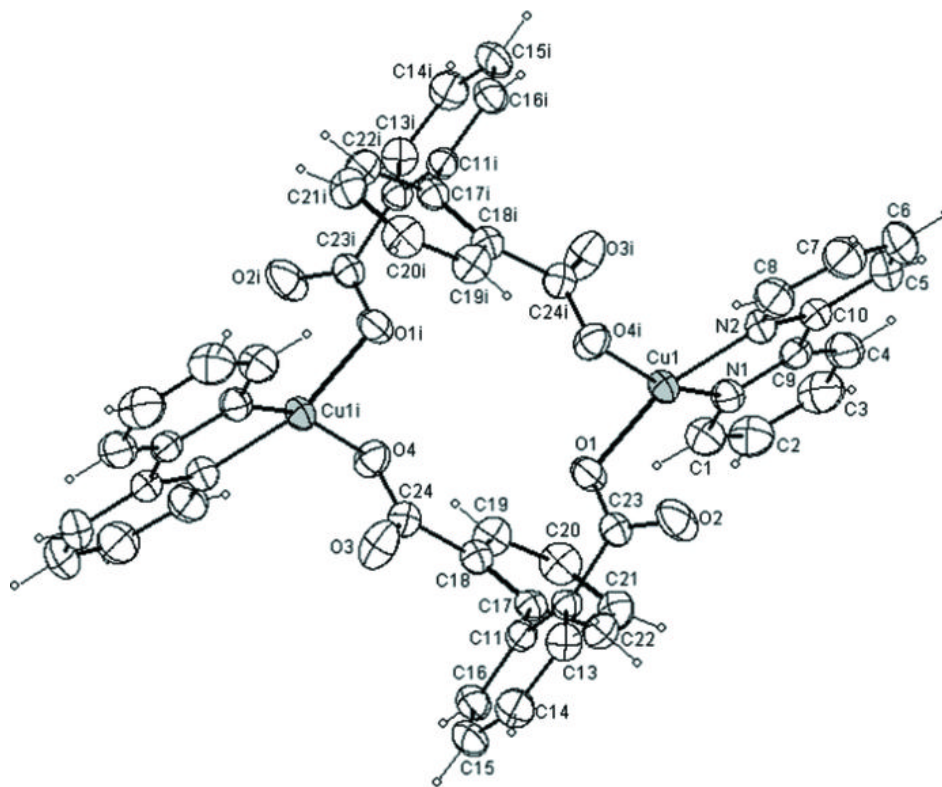


Fig. 2

