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Tetra-μ-acetato-bis{[*N*-(4-methylphenyl)-pyridine-3-carboxamide]copper(II)} ethanol disolvate

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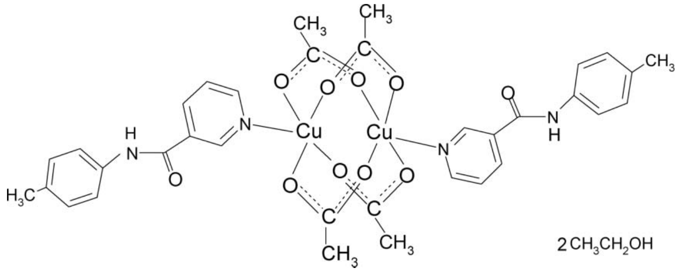
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.089; data-to-parameter ratio = 14.7.

The title compound, $[Cu_2(C_2H_3O_2)_4(C_{13}H_{12}N_2O)_2]\cdot 2C_2H_5OH$, contains a centrosymmetric dinuclear copper(II) unit bridged by four acetate groups with two pyridine amide ligands occupying the axial positions. Each Cu atom is in a square-pyramidal coordination environment, and is displaced from the basal plane of the O atoms by 0.2071 (3) Å towards the pyridine nitrogen. The Cu$\cdots$Cu separation is 2.6442 (5) Å. The amide groups of the ligands participate in the formation of intermolecular hydrogen bonds. Hydrogen bonds and π–π interactions between the pyridyl and benzene rings of neighbouring molecules [centroid-to-centroid distance 3.640 (4) Å] generate a two-dimensional supramolecular network.

Related literature

For general background, see: Kitagawa *et al.* (2004); Whitesides & Grzybowski (2002); James (2003); Evans & Lin (2002). For related structures, see: Clement *et al.* (1998); Noveron *et al.* (2002); Belda & Moberg (2005); Ge *et al.* (2005).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{13}H_{12}N_2O)_2]$·$2C_2H_6O$
M_r = 879.88
Triclinic, $P\bar{1}$
a = 8.3874 (6) Å
b = 8.9727 (7) Å
c = 13.4394 (10) Å
α = 87.5385 (10)°
β = 84.0111 (11)°
γ = 87.8028 (11)°
V = 1004.38 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 295 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.764, T_{max} = 0.817
5652 measured reflections
3863 independent reflections
3592 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.089
S = 1.08
3863 reflections
262 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
C1—H1$\cdots$O1	0.93	2.42	2.758 (3)	101
C5—H5$\cdots$O4	0.93	2.43	3.029 (3)	122
C8—H8$\cdots$O1	0.93	2.27	2.863 (3)	121
C3—H3$\cdots$O6^{i}	0.93	2.31	3.231 (3)	175
C12—H12$\cdots$O6^{i}	0.93	2.54	3.350 (3)	146
O6—H20$\cdots$O3^{ii}	0.82	2.04	2.850 (2)	171
N2—H2$\cdots$O6^{i}	0.83 (2)	2.29 (2)	3.108 (2)	165.9 (18)

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2147).

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supplementary materials

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Tetra-μ-acetato-bis{[*N*-(4-methylphenyl)pyridine-3-carboxamide]copper(II)} ethanol disolvate

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Comment

Recently, there has been growing interest in the rational design and construction of supramolecular architectures based on metal-organic frameworks with weak non-covalent interactions, such as hydrogen bonding and π-π stacking interactions (Kitagawa *et al.*, 2004; Whitesides & Grzybowski, 2002; James, 2003; Evans & Lin, 2002). The amide group can be either hydrogen bonding donor or acceptor to form intra- or intermolecular hydrogen bonds. It can be further used to construct supramolecular coordination networks. During the past decade, various types of pyridine amide ligands and their compounds with transition metals have been synthesized (see, for example, Clement *et al.*, 1998; Noveron *et al.*, 2002; Belda & Moberg, 2005). As far as we know, among the studies on transition metal-pyridinecarboxamide coordination compounds, most ligands are chelating bidentate 2-pyridinecarboxamide derivatives but few are concerned with non-chelation-controlled 3- or 4-pyridinecarboxamide groups (see, for example, Ge *et al.*, 2005). In this paper, the crystal structure of the title copper(II) dinuclear complex is reported.

The title compound consists of centrosymmetric [$Cu_2(\mu\text{-}CH_3COO)_4$] units with a geometry similar to that of other copper acetate derivatives. Coordination around the metal centre includes four oxygen atoms (O2, O3, O4 and O5) from four different acetate groups in a basal plane, while the axial site is occupied by a pyridine amide ligand coordinated through the pyridine nitrogen atom (Fig.1). As a result, each Cu^{II} atom presents a distorted square pyramidal geometry. The average value of the Cu—O bond distances is 1.976 (2) Å. The copper atom is displaced from the basal plane to the apical N atom by 0.2071 (3) Å. The Cu···Cu seperation is 2.6442 (5) Å. The amide groups of the ligands and the hydroxy groups of the solvate molecules are involved in the formation of intermolecular hydrogen bonds (Table 1) to give one-dimensional chains. The chains are further stacked through face-to-face π–π interactions occurring between the pyridyl and phenyl rings of centrosymmetrically related molecules ($Cg1\cdots Cg2_i$ = 3.640 (4) Å; *Cg*1 and *Cg*2 are the centroids of the pyridyl and benzene rings, respectively; symmetry code: (i) $1 - x, -y, 1 - z$) to generate a two-dimensional network (Fig.2).

Experimental

N-(4-methylphenyl)-3-pyridinecarboxamide was prepared by reaction of nicotinoyl chloride hydrochloride and 4-methylaniline in the presence of triethylamine, similarly to the literature method (Noveron *et al.*, 2002). An ethanolic solution of the organic ligand (0.5 mmol in 20 ml e thanol) was added dropwise to $Cu(OAc)_2$ (0.5 mmol in 5 ml e thanol) with stirring. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent at room temperature.

Refinement

The H atom bound to the N atom was located in a difference Fourier map and refined with a distance restraint of 0.87 (2) Å. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å, O—H = 0.84 Å and with $U_{iso}(H) = 1.2\ U_{eq}(C)$ or $1.5\ U_{eq}(C, O)$ for methyl and hydroxy groups.

Figures

Fig. 1. The molecular structure of title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms and ethanol molecules have been omitted for clarity. Unlabelled atoms or labelled with the suffix A are generated by the symmetry operation (−*x*, −*y*, −*z*).

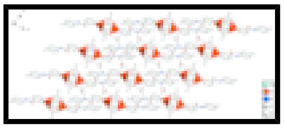

Fig. 2. Packing diagram of the title compound viewed along the *b* axis, with H atoms are omitted for clarity. Hydrogen bonds are indicated as dashed lines, π-π interactions are shown as double arrows.

Tetra-μ-acetato-bis{[*N*-(4-methylphenyl)pyridine-3-\ carboxamide]copper(II)} ethanol disolvate

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{13}H_{12}N_2O)_2]\cdot 2C_2H_6O$	$Z = 1$
$M_r = 879.88$	$F_{000} = 458$
Triclinic, $P\overline{1}$	$D_x = 1.455$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
a = 8.3874 (6) Å	Cell parameters from 857 reflections
b = 8.9727 (7) Å	θ = 2.7–22.7°
c = 13.4394 (10) Å	μ = 1.13 mm^{-1}
α = 87.5385 (10)°	*T* = 295 (2) K
β = 84.0111 (11)°	Block, green
γ = 87.8028 (11)°	0.24 × 0.22 × 0.18 mm
V = 1004.38 (13) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3863 independent reflections
Radiation source: fine-focus sealed tube	3592 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.012$
T = 295(2) K	$\theta_{max} = 26.0°$
φ and ω scans	$\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 7$
$T_{min} = 0.764$, $T_{max} = 0.817$	$k = -11 \rightarrow 11$
5652 measured reflections	$l = -13 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.6567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.002$
3863 reflections	$\Delta\rho_{max} = 0.80$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.04088 (3)	−0.01389 (3)	0.092416 (17)	0.02796 (10)
O3	−0.17511 (18)	0.08329 (18)	0.12550 (11)	0.0351 (3)
O2	−0.24597 (19)	0.0984 (2)	−0.03016 (12)	0.0426 (4)
O4	−0.0597 (2)	−0.20760 (18)	0.08519 (12)	0.0405 (4)
N1	0.0854 (2)	−0.05405 (19)	0.24740 (12)	0.0276 (4)
O5	−0.1308 (2)	−0.18505 (19)	−0.07058 (12)	0.0401 (4)
C7	0.4107 (2)	0.1781 (2)	0.59872 (15)	0.0271 (4)
N2	0.3303 (2)	0.0881 (2)	0.53644 (13)	0.0277 (4)
C2	0.2010 (2)	0.0074 (2)	0.39562 (14)	0.0274 (4)
C16	−0.2730 (3)	0.1171 (2)	0.06194 (15)	0.0310 (4)
C14	−0.1247 (3)	−0.2537 (2)	0.01231 (16)	0.0324 (5)
C3	0.1349 (3)	−0.1172 (2)	0.44608 (15)	0.0309 (4)
H3	0.1512	−0.1388	0.5126	0.037*
C10	0.5679 (3)	0.3390 (2)	0.73204 (17)	0.0334 (5)
O1	0.3362 (3)	0.2339 (2)	0.39399 (14)	0.0663 (7)
C4	0.0438 (3)	−0.2090 (2)	0.39560 (16)	0.0347 (5)
H4	−0.0014	−0.2934	0.4278	0.042*
C1	0.1730 (3)	0.0336 (2)	0.29597 (15)	0.0296 (4)
H1	0.2177	0.1166	0.2616	0.036*
C15	−0.2020 (3)	−0.4033 (3)	0.0268 (2)	0.0462 (6)
H14A	−0.1494	−0.4638	0.0751	0.069*
H14B	−0.1923	−0.4522	−0.0358	0.069*
H14C	−0.3133	−0.3890	0.0503	0.069*
C5	0.0213 (3)	−0.1737 (2)	0.29731 (15)	0.0315 (4)

H5	−0.0409	−0.2351	0.2642	0.038*
C8	0.4870 (3)	0.3079 (3)	0.56612 (18)	0.0389 (5)
H8	0.4869	0.3425	0.4999	0.047*
C12	0.4136 (3)	0.1294 (3)	0.69781 (16)	0.0394 (5)
H12	0.3625	0.0424	0.7208	0.047*
C9	0.5641 (3)	0.3865 (3)	0.63337 (19)	0.0420 (6)
H9	0.6146	0.4740	0.6109	0.050*
C17	−0.4343 (3)	0.1845 (3)	0.09855 (19)	0.0461 (6)
H17A	−0.4458	0.1833	0.1704	0.069*
H17B	−0.5172	0.1276	0.0759	0.069*
H17C	−0.4428	0.2856	0.0727	0.069*
C6	0.2965 (3)	0.1202 (2)	0.44166 (16)	0.0338 (5)
C13	0.6533 (3)	0.4252 (3)	0.8036 (2)	0.0449 (6)
H13A	0.7017	0.5103	0.7687	0.067*
H13B	0.7349	0.3620	0.8302	0.067*
H13C	0.5775	0.4580	0.8574	0.067*
C11	0.4920 (3)	0.2090 (3)	0.76295 (17)	0.0412 (6)
H11	0.4933	0.1740	0.8290	0.049*
O6	0.2147 (2)	0.81818 (18)	0.67434 (12)	0.0449 (4)
H20	0.1936	0.8498	0.7307	0.067*
C18	0.2257 (4)	0.6616 (3)	0.6802 (3)	0.0630 (8)
H18A	0.2969	0.6297	0.7300	0.076*
H18B	0.2720	0.6256	0.6162	0.076*
C19	0.0700 (7)	0.5953 (5)	0.7065 (4)	0.1196 (19)
H19A	0.0283	0.6229	0.7726	0.179*
H19B	0.0822	0.4886	0.7046	0.179*
H19C	−0.0028	0.6308	0.6595	0.179*
H2	0.302 (3)	0.007 (2)	0.5640 (17)	0.029 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02822 (15)	0.03793 (16)	0.01920 (14)	−0.00463 (10)	−0.00729 (10)	−0.00319 (10)
O3	0.0315 (8)	0.0495 (9)	0.0241 (7)	0.0022 (7)	−0.0038 (6)	−0.0010 (6)
O2	0.0326 (8)	0.0676 (11)	0.0282 (8)	0.0085 (8)	−0.0078 (6)	−0.0057 (7)
O4	0.0546 (10)	0.0393 (9)	0.0312 (8)	−0.0126 (7)	−0.0162 (7)	−0.0030 (7)
N1	0.0277 (9)	0.0334 (9)	0.0227 (8)	−0.0031 (7)	−0.0061 (7)	−0.0018 (7)
O5	0.0461 (9)	0.0471 (9)	0.0303 (8)	−0.0173 (7)	−0.0123 (7)	−0.0035 (7)
C7	0.0265 (10)	0.0318 (10)	0.0246 (10)	−0.0020 (8)	−0.0078 (8)	−0.0059 (8)
N2	0.0330 (9)	0.0289 (9)	0.0229 (8)	−0.0083 (7)	−0.0089 (7)	−0.0003 (7)
C2	0.0284 (10)	0.0331 (10)	0.0217 (9)	−0.0020 (8)	−0.0067 (8)	−0.0033 (8)
C16	0.0302 (11)	0.0357 (11)	0.0276 (10)	−0.0034 (9)	−0.0045 (8)	−0.0002 (8)
C14	0.0296 (11)	0.0377 (11)	0.0313 (11)	−0.0053 (9)	−0.0063 (8)	−0.0072 (9)
C3	0.0389 (12)	0.0341 (11)	0.0215 (9)	−0.0035 (9)	−0.0103 (8)	−0.0005 (8)
C10	0.0303 (11)	0.0356 (11)	0.0366 (12)	−0.0002 (9)	−0.0103 (9)	−0.0110 (9)
O1	0.1108 (18)	0.0575 (12)	0.0392 (10)	−0.0492 (12)	−0.0395 (11)	0.0178 (9)
C4	0.0456 (13)	0.0314 (11)	0.0288 (11)	−0.0099 (9)	−0.0093 (9)	0.0023 (9)
C1	0.0324 (11)	0.0347 (11)	0.0225 (10)	−0.0053 (9)	−0.0059 (8)	0.0021 (8)

C15	0.0516 (15)	0.0421 (13)	0.0480 (14)	−0.0145 (11)	−0.0136 (12)	−0.0043 (11)
C5	0.0351 (11)	0.0337 (11)	0.0280 (10)	−0.0049 (9)	−0.0101 (9)	−0.0053 (8)
C8	0.0464 (13)	0.0398 (12)	0.0339 (12)	−0.0128 (10)	−0.0186 (10)	0.0056 (9)
C12	0.0518 (14)	0.0428 (12)	0.0262 (11)	−0.0213 (11)	−0.0094 (10)	0.0013 (9)
C9	0.0473 (14)	0.0354 (12)	0.0471 (14)	−0.0126 (10)	−0.0207 (11)	0.0046 (10)
C17	0.0365 (13)	0.0604 (16)	0.0405 (13)	0.0082 (11)	−0.0035 (10)	−0.0022 (11)
C6	0.0408 (12)	0.0364 (11)	0.0262 (10)	−0.0103 (9)	−0.0105 (9)	0.0004 (9)
C13	0.0452 (14)	0.0455 (14)	0.0482 (14)	−0.0065 (11)	−0.0165 (11)	−0.0178 (11)
C11	0.0514 (14)	0.0501 (14)	0.0246 (11)	−0.0151 (11)	−0.0103 (10)	−0.0034 (10)
O6	0.0689 (12)	0.0384 (9)	0.0287 (8)	−0.0104 (8)	−0.0081 (8)	−0.0019 (7)
C18	0.084 (2)	0.0405 (15)	0.0635 (19)	0.0048 (14)	−0.0047 (16)	−0.0034 (13)
C19	0.168 (5)	0.070 (3)	0.128 (4)	−0.062 (3)	−0.034 (4)	0.013 (3)

Geometric parameters (Å, °)

Cu1—O5^{i}	1.9629 (16)	O1—C6	1.219 (3)
Cu1—O4	1.9712 (16)	C4—C5	1.376 (3)
Cu1—O2^{i}	1.9717 (16)	C4—H4	0.9300
Cu1—O3	1.9960 (15)	C1—H1	0.9300
Cu1—N1	2.1669 (17)	C15—H14A	0.9600
Cu1—Cu1^{i}	2.6442 (5)	C15—H14B	0.9600
O3—C16	1.265 (3)	C15—H14C	0.9600
O2—C16	1.252 (3)	C5—H5	0.9300
O2—Cu1^{i}	1.9717 (16)	C8—C9	1.394 (3)
O4—C14	1.261 (3)	C8—H8	0.9300
N1—C1	1.331 (3)	C12—C11	1.385 (3)
N1—C5	1.341 (3)	C12—H12	0.9300
O5—C14	1.254 (3)	C9—H9	0.9300
O5—Cu1^{i}	1.9629 (16)	C17—H17A	0.9600
C7—C8	1.383 (3)	C17—H17B	0.9600
C7—C12	1.386 (3)	C17—H17C	0.9600
C7—N2	1.423 (2)	C13—H13A	0.9600
N2—C6	1.350 (3)	C13—H13B	0.9600
N2—H2	0.831 (16)	C13—H13C	0.9600
C2—C3	1.386 (3)	C11—H11	0.9300
C2—C1	1.392 (3)	O6—C18	1.404 (3)
C2—C6	1.506 (3)	O6—H20	0.8200
C16—C17	1.504 (3)	C18—C19	1.459 (6)
C14—C15	1.509 (3)	C18—H18A	0.9700
C3—C4	1.388 (3)	C18—H18B	0.9700
C3—H3	0.9300	C19—H19A	0.9600
C10—C11	1.378 (3)	C19—H19B	0.9600
C10—C9	1.379 (3)	C19—H19C	0.9600
C10—C13	1.512 (3)		
O5^{i}—Cu1—O4	168.04 (6)	C14—C15—H14A	109.5
O5^{i}—Cu1—O2^{i}	88.33 (8)	C14—C15—H14B	109.5
O4—Cu1—O2^{i}	90.30 (8)	H14A—C15—H14B	109.5

O5^{i}—Cu1—O3	88.91 (7)	C14—C15—H14C	109.5
O4—Cu1—O3	89.94 (7)	H14A—C15—H14C	109.5
O2^{i}—Cu1—O3	167.81 (6)	H14B—C15—H14C	109.5
O5^{i}—Cu1—N1	98.67 (6)	N1—C5—C4	122.55 (19)
O4—Cu1—N1	93.29 (6)	N1—C5—H5	118.7
O2^{i}—Cu1—N1	97.74 (6)	C4—C5—H5	118.7
O3—Cu1—N1	94.41 (6)	C7—C8—C9	119.5 (2)
O5^{i}—Cu1—Cu1^{i}	87.25 (5)	C7—C8—H8	120.3
O4—Cu1—Cu1^{i}	80.79 (5)	C9—C8—H8	120.3
O2^{i}—Cu1—Cu1^{i}	85.24 (5)	C11—C12—C7	120.6 (2)
O3—Cu1—Cu1^{i}	82.77 (4)	C11—C12—H12	119.7
N1—Cu1—Cu1^{i}	173.42 (5)	C7—C12—H12	119.7
C16—O3—Cu1	124.23 (14)	C10—C9—C8	122.2 (2)
C16—O2—Cu1^{i}	122.86 (14)	C10—C9—H9	118.9
C14—O4—Cu1	126.81 (15)	C8—C9—H9	118.9
C1—N1—C5	118.08 (17)	C16—C17—H17A	109.5
C1—N1—Cu1	123.62 (14)	C16—C17—H17B	109.5
C5—N1—Cu1	118.30 (13)	H17A—C17—H17B	109.5
C14—O5—Cu1^{i}	119.77 (14)	C16—C17—H17C	109.5
C8—C7—C12	118.82 (19)	H17A—C17—H17C	109.5
C8—C7—N2	124.23 (18)	H17B—C17—H17C	109.5
C12—C7—N2	116.95 (19)	O1—C6—N2	123.9 (2)
C6—N2—C7	127.68 (18)	O1—C6—C2	119.83 (19)
C6—N2—H2	118.9 (17)	N2—C6—C2	116.22 (18)
C7—N2—H2	113.4 (17)	C10—C13—H13A	109.5
C3—C2—C1	117.91 (19)	C10—C13—H13B	109.5
C3—C2—C6	124.80 (18)	H13A—C13—H13B	109.5
C1—C2—C6	117.26 (19)	C10—C13—H13C	109.5
O2—C16—O3	124.8 (2)	H13A—C13—H13C	109.5
O2—C16—C17	116.93 (19)	H13B—C13—H13C	109.5
O3—C16—C17	118.28 (19)	C10—C11—C12	121.5 (2)
O5—C14—O4	125.3 (2)	C10—C11—H11	119.3
O5—C14—C15	117.69 (19)	C12—C11—H11	119.3
O4—C14—C15	117.0 (2)	C18—O6—H20	109.5
C2—C3—C4	118.87 (19)	O6—C18—C19	112.4 (3)
C2—C3—H3	120.6	O6—C18—H18A	109.1
C4—C3—H3	120.6	C19—C18—H18A	109.1
C11—C10—C9	117.4 (2)	O6—C18—H18B	109.1
C11—C10—C13	121.1 (2)	C19—C18—H18B	109.1
C9—C10—C13	121.4 (2)	H18A—C18—H18B	107.8
C5—C4—C3	119.2 (2)	C18—C19—H19A	109.5
C5—C4—H4	120.4	C18—C19—H19B	109.5
C3—C4—H4	120.4	H19A—C19—H19B	109.5
N1—C1—C2	123.39 (19)	C18—C19—H19C	109.5
N1—C1—H1	118.3	H19A—C19—H19C	109.5
C2—C1—H1	118.3	H19B—C19—H19C	109.5

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.93	2.42	2.758 (3)	101
C5—H5···O4	0.93	2.43	3.029 (3)	122
C8—H8···O1	0.93	2.27	2.863 (3)	121
C3—H3···O6^{ii}	0.93	2.31	3.231 (3)	175
C12—H12···O6^{ii}	0.93	2.54	3.350 (3)	146
O6—H20···O3^{iii}	0.82	2.04	2.850 (2)	171
N2—H2···O6^{ii}	0.83 (2)	2.29 (2)	3.108 (2)	165.9 (18)

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

Fig. 1

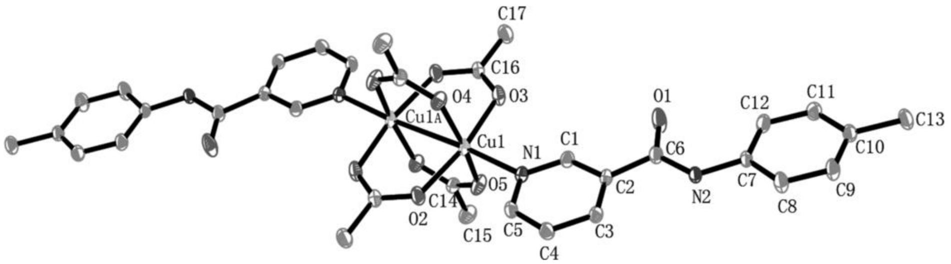
C17
C16
O4
O3
Cu1A
Cu1
N1
C1
O1
C6
C12
C11
C13
C10
C2
N2
C7
C9
C8
O5
C14
O2
C15
C5
C4
C3

Fig. 2