Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4,4′-Dimethoxy-2,2′-[ethylenedioxybis(nitrilomethylidyne)]diphenolato}copper(II)

Yin-Xia Sun,[a] Su-Xia Gao,[b] Jun-Yan Shi[a] and Wen-Kui Dong[a]*

[a]School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, People's Republic of China, and [b]School of Environmental Science and Municipal Engineering, Lanzhou Jiaotong University, Lanzhou 730070, People's Republic of China
Correspondence e-mail: dongwk@mail.lzjtu.cn

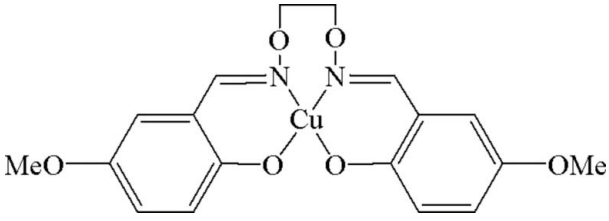
Received 10 July 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.082; data-to-parameter ratio = 12.8.

The title complex, $[Cu(C_{18}H_{18}N_2O_6)]$, was synthesized by the reaction of copper(II) acetate monohydrate with the ligand 4,4′-dimethoxy-2,2′-[ethylenedioxybis(nitrilomethylidyne)]-diphenol (H_2L). The Cu atom is coordinated by two O atoms and two N atoms of the L^{2-} unit. A bridged dimer is formed through intermolecular Cu···O interactions [Cu···O = 1.9408 (15) Å], creating a distorted square-pyramidal geometry about the Cu atoms.

Related literature

For related literature, see: Akine *et al.* (2001, 2005); Bhadbhade & Srinivas (1993); Garnovskii *et al.* (1993); Katsuki (1995); Ray *et al.* (2003); Sun *et al.* (2004); Sangeetha *et al.* (1999).



Experimental

Crystal data

$[Cu(C_{18}H_{18}N_2O_6)]$
M_r = 421.88
Monoclinic, $P2_1/c$
a = 15.453 (2) Å
b = 7.6408 (11) Å
c = 15.927 (2) Å
β = 107.686 (2)°
V = 1791.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 298 (2) K
0.51 × 0.29 × 0.20 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1996)
T_{min} = 0.566, T_{max} = 0.787
8649 measured reflections
3138 independent reflections
2600 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.10
3138 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of Gansu (grant No. 0604-01) and the Graduate Students Science Innovation Fund (grant No. DXS-2006-80) of Lanzhou Jiaotong University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2018).

References

Akine, S., Takanori, T., Taniguchi, T. & Nabeshima, T. (2005). *Inorg. Chem.* **44**, 3270–3274.
Akine, S., Taniguchi, T. & Nabeshima, T. (2001). *Chem. Lett.* pp. 682–683.
Bhadbhade, M. M. & Srinivas, D. (1993). *Inorg. Chem.* **32**, 6122–6125.
Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1996). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Garnovskii, A. D., Nivorozkhin, A. L. & Minkin, V. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Katsuki, T. (1995). *Coord. Chem. Rev.* **140**, 189–214.
Ray, M. S., Mukhopadhyay, G. M., Drew, M. G. B., Lu, T. H., Chaudhuri, S. & Ghosh, A. (2003). *Inorg. Chem. Commun.* **6**, 961–965.
Sangeetha, N. R., Barradi, K., Gupta, C. K., Pal, V. & Manivannan, S. P. (1999). *Polyhedron*, **18**, 1425–1429.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997*a*). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sun, S. S., Stern, C. L., Nguyen, S. T. & Hupp, J. T. (2004). *J. Am. Chem. Soc.* **126**, 6314–6326.

  doi:10.1107/S1600536807061752

supplementary materials

Acta Cryst. (2008). E**64**, m226 [**doi:10.1107/S1600536807061752**]

{4,4'-Dimethoxy-2,2'-[ethylenedioxybis(nitrilomethylidyne)]diphenolato}copper(II)

Y.-X. Sun, S.-X. Gao, J.-Y. Shi and W.-K. Dong

Comment

Metal complexes with multidentate salen-type ligands have been extensively studied because such ligands can bind with one, two, or more metal centers involving various modes and allow successful synthesis of homo and/or heteronuclear metal complexes with interesting stereochemistry (Katsuki, 1995; Akine *et al.*, 2005). Furthermore, these complexes are very interesting in many fields, such as catalysis, enzymatic reactions (Garnovskii *et al.*, 1993), magnetism, and molecular architectures(Sun *et al.*, 2004). Research into the copper(II) complexes have been stimulated by, among other things, biological modeling applications, catalysis, design of molecular ferromagnets, and material chemistry (Ray *et al.*, 2003).

In this paper, a novel salen-type bisoxime chelating ligand, 4,4'-dimethoxy-2,2'-[ethylenedioxybis(nitrilomethylidyne)]diphenol, and its mononuclear copper(II) complex, (I), were synthesized. The X-ray crystallography of the title complex reveals the complex crystallizes in the monoclinic system, space group P2(1)/c with a = 15.453 (2) Å, b = 7.6408 (11) Å, c = 15.927 (2) Å, β = 107.686 (2) ° and *Z* = 4. The copper(II) atom has a tetragonally elongated square-pyramidal configuration with donor atoms O3, O5, N1, and N2 (Cu1—O3: 1.9408 (15) Å; Cu1—O5: 1.9068 (17) Å; Cu1—N1: 2.032 (2) Å; Cu1—N2: 1.9670 (19) Å) forming a near-perfect basal plane and the apical bond Cu1···O3A (2.411 (2) Å) being almost perpendicular to this plane. The copper(II) atom is displaced by 0.164 Å toward the bridging oxygen O3A from the best plane of the donor atoms. The dihedral angle between the coordination plane of O3—Cu1—N1 and that of O5—Cu1—N2 is 15.46 °, indicating slight distortion toward tetrahedral geometry from the square planar structure. The title complex has a stepped conformation as observed in the dimers of [Cu(salamo)] (Akine *et al.*, 2001) and [Cu(salen)] (Bhadbhade & Srinivas, 1993), which forms a head-to-tail structure by the intermolecular contacts between copper(II) and oxygen atoms(Fig. 2). The bond angles related to Cu2O2 are as follows: the angles of O3—Cu1—O3A and O3—Cu1A—O3A are both 85.15 °, the angles of Cu1—O3—Cu1A and Cu1—O3A—Cu1A are the same as 94.85 °. All of the Cu1—O—Cu1A bridging angles fall in the normal range for diphenoxo-bridged copper(II) complexes (Sangeetha *et al.*, 1999). The sum of the four bond angles is 360 ° exactly, indicating Cu1, O3, Cu1A and O3A are coplanar. The Cu1—Cu1A distance in dimer is 3.245 (2) Å.

Experimental

A solution of Cu(II) acetate monohydrate (6.7 mg, 0.03 mmol) in ethanol (2 ml) was added dropwise to a solution of 4,4'-dimethoxy-2,2'-[ethylenedioxybis(nitrilomethylidyne)]diphenol (12 mg, 0.03 mmol) in acetone (10 ml). The color of the mixing solution turns to green, immediately, and then filtering the solution and the filtrate was allowed to stand at room temperature for about two weeks, the solvent was partially evaporated and obtained dark-brown prismatic single crystals suitable for X-ray crystallographic analysis.

Refinement

Non-H atoms were refined anisotropically. H atoms were treated as riding atoms with distances C—H = 0.97 (CH_2), or 0.93 Å (CH),*O*—H = 0.82 Å, and U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(O).

Figures

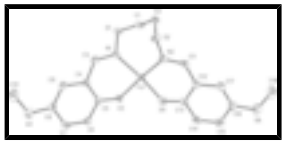


Fig. 1. The molecule structure (I) with atom numbering. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

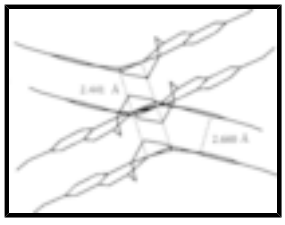


Fig. 2. Crystal structure of the title complex showing the formation of a dimer. Distances of Cu1···O3A [2.411 (2) Å] and pi-pi interactions [2.660 (2) Å].

{4,4'-Dimethoxy-2,2'- [ethylenedioxybis(nitrilomethylidyne)]diphenolato}copper(II)

Crystal data

$[Cu(C_{18}H_{18}N_2O_6)]$	$F(000)$ = 868
M_r = 421.88	D_x = 1.564 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 15.453 (2) Å	Cell parameters from 4146 reflections
b = 7.6408 (11) Å	θ = 2.6–28.2°
c = 15.927 (2) Å	μ = 1.26 mm^{-1}
β = 107.686 (2)°	T = 298 K
V = 1791.6 (4) Å^3	Prismatic, brown
Z = 4	0.51 × 0.29 × 0.20 mm

Data collection

Bruker APEX CCD area-detector diffractometer	3138 independent reflections
Radiation source: fine-focus sealed tube	2600 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.027
φ and ω scans	θ_{max} = 25.0°, θ_{min} = 2.6°
Absorption correction: multi-scan (*SADABS*; Bruker, 2000?)	h = −18→17
T_{min} = 0.566, T_{max} = 0.787	k = −9→9
8649 measured reflections	l = −11→18

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.082$	H-atom parameters constrained
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.4958P]$ where $P = (F_o^2 + 2F_c^2)/3$
3138 reflections	$(\Delta/\sigma)_{max} = 0.001$
246 parameters	$\Delta\rho_{max} = 0.25$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.40$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.477290 (19)	−0.02861 (4)	0.592030 (18)	0.03177 (12)
N1	0.58032 (14)	−0.2027 (3)	0.63744 (13)	0.0346 (5)
N2	0.39767 (13)	−0.1437 (3)	0.65094 (12)	0.0322 (5)
O1	0.57217 (12)	−0.3861 (2)	0.64483 (13)	0.0489 (5)
O2	0.43329 (12)	−0.2799 (2)	0.71371 (10)	0.0390 (4)
O3	0.56375 (10)	0.1234 (2)	0.56144 (10)	0.0328 (4)
O4	0.91554 (12)	0.2546 (3)	0.76874 (13)	0.0552 (5)
O5	0.39007 (11)	0.1542 (2)	0.55425 (11)	0.0393 (4)
O6	0.03883 (14)	0.2491 (3)	0.56161 (17)	0.0680 (6)
C1	0.48180 (17)	−0.4460 (3)	0.60408 (17)	0.0406 (6)
H1A	0.4833	−0.5640	0.5821	0.049*
H1B	0.4523	−0.3711	0.5544	0.049*
C2	0.42871 (18)	−0.4441 (3)	0.66883 (17)	0.0400 (6)
H2A	0.3656	−0.4704	0.6379	0.048*
H2B	0.4516	−0.5356	0.7121	0.048*
C3	0.66344 (17)	−0.1582 (3)	0.67144 (17)	0.0380 (6)
H3	0.7040	−0.2446	0.7003	0.046*
C4	0.69934 (17)	0.0146 (3)	0.66865 (16)	0.0344 (6)

C5	0.64843 (15)	0.1439 (3)	0.61155 (15)	0.0307 (5)
C6	0.69354 (16)	0.3032 (3)	0.60920 (16)	0.0359 (6)
H6	0.6629	0.3910	0.5713	0.043*
C7	0.78087 (17)	0.3335 (4)	0.66068 (17)	0.0402 (6)
H7	0.8081	0.4405	0.6569	0.048*
C8	0.82935 (16)	0.2064 (4)	0.71851 (17)	0.0385 (6)
C9	0.78927 (17)	0.0474 (3)	0.72178 (17)	0.0390 (6)
H9	0.8216	−0.0394	0.7593	0.047*
C10	0.9674 (2)	0.1302 (5)	0.8288 (2)	0.0790 (11)
H10A	0.9378	0.1040	0.8723	0.118*
H10B	1.0267	0.1769	0.8573	0.118*
H10C	0.9728	0.0252	0.7977	0.118*
C11	0.31864 (17)	−0.0951 (3)	0.65357 (16)	0.0365 (6)
H11	0.2925	−0.1587	0.6894	0.044*
C12	0.26844 (17)	0.0485 (3)	0.60588 (16)	0.0356 (6)
C13	0.30721 (16)	0.1661 (3)	0.55881 (15)	0.0343 (6)
C14	0.25243 (17)	0.3072 (3)	0.51642 (18)	0.0428 (6)
H14	0.2758	0.3865	0.4847	0.051*
C15	0.16610 (18)	0.3314 (4)	0.52042 (18)	0.0455 (7)
H15	0.1325	0.4275	0.4926	0.055*
C16	0.12811 (18)	0.2130 (4)	0.56585 (19)	0.0468 (7)
C17	0.17833 (18)	0.0747 (4)	0.60834 (19)	0.0448 (7)
H17	0.1533	−0.0034	0.6393	0.054*
C18	−0.0041 (2)	0.1304 (6)	0.6035 (3)	0.0805 (11)
H18A	−0.0043	0.0160	0.5785	0.121*
H18B	−0.0654	0.1676	0.5953	0.121*
H18C	0.0282	0.1265	0.6653	0.121*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03453 (18)	0.02879 (19)	0.03462 (18)	−0.00140 (12)	0.01445 (13)	0.00478 (13)
N1	0.0442 (12)	0.0240 (11)	0.0385 (11)	0.0009 (9)	0.0168 (10)	0.0044 (9)
N2	0.0400 (12)	0.0291 (11)	0.0285 (10)	−0.0012 (9)	0.0121 (9)	0.0061 (8)
O1	0.0487 (11)	0.0240 (10)	0.0756 (14)	0.0007 (8)	0.0214 (10)	0.0039 (9)
O2	0.0503 (11)	0.0383 (10)	0.0293 (9)	0.0032 (8)	0.0134 (8)	0.0098 (8)
O3	0.0297 (9)	0.0335 (10)	0.0346 (9)	−0.0040 (7)	0.0087 (7)	0.0067 (7)
O4	0.0374 (10)	0.0574 (13)	0.0605 (13)	−0.0028 (9)	−0.0005 (9)	−0.0010 (10)
O5	0.0391 (10)	0.0341 (10)	0.0492 (10)	0.0004 (8)	0.0200 (8)	0.0108 (8)
O6	0.0435 (12)	0.0683 (15)	0.0981 (17)	0.0101 (10)	0.0303 (12)	0.0139 (13)
C1	0.0563 (17)	0.0255 (14)	0.0393 (15)	−0.0066 (12)	0.0133 (13)	−0.0008 (11)
C2	0.0448 (15)	0.0320 (15)	0.0406 (14)	−0.0043 (11)	0.0091 (12)	0.0109 (11)
C3	0.0418 (15)	0.0312 (14)	0.0419 (14)	0.0063 (11)	0.0139 (12)	0.0064 (11)
C4	0.0382 (14)	0.0315 (14)	0.0361 (13)	0.0025 (10)	0.0150 (11)	0.0008 (11)
C5	0.0327 (13)	0.0320 (14)	0.0307 (12)	0.0004 (10)	0.0145 (10)	−0.0011 (10)
C6	0.0341 (13)	0.0335 (14)	0.0398 (14)	−0.0005 (11)	0.0107 (11)	0.0082 (11)
C7	0.0375 (14)	0.0357 (15)	0.0492 (16)	−0.0058 (11)	0.0159 (12)	−0.0001 (12)
C8	0.0297 (13)	0.0452 (16)	0.0397 (14)	−0.0004 (11)	0.0094 (11)	−0.0056 (12)

C9	0.0379 (14)	0.0384 (16)	0.0388 (14)	0.0083 (11)	0.0089 (11)	0.0040 (11)
C10	0.0525 (19)	0.085 (3)	0.078 (2)	−0.0001 (18)	−0.0126 (18)	0.013 (2)
C11	0.0413 (15)	0.0361 (15)	0.0359 (14)	−0.0056 (11)	0.0175 (12)	0.0042 (11)
C12	0.0367 (13)	0.0349 (15)	0.0359 (13)	−0.0037 (11)	0.0122 (11)	−0.0007 (11)
C13	0.0364 (13)	0.0329 (14)	0.0323 (13)	−0.0056 (11)	0.0086 (11)	−0.0012 (11)
C14	0.0418 (15)	0.0362 (15)	0.0478 (16)	−0.0037 (12)	0.0097 (12)	0.0091 (12)
C15	0.0411 (15)	0.0378 (16)	0.0508 (16)	0.0015 (12)	0.0040 (13)	0.0031 (13)
C16	0.0350 (14)	0.0495 (18)	0.0562 (17)	−0.0001 (12)	0.0145 (13)	−0.0043 (14)
C17	0.0425 (15)	0.0445 (17)	0.0513 (16)	−0.0038 (12)	0.0204 (13)	0.0047 (13)
C18	0.058 (2)	0.090 (3)	0.110 (3)	0.0051 (19)	0.052 (2)	0.010 (2)

Geometric parameters (Å, °)

Cu1—O5	1.9068 (17)	C5—C6	1.409 (3)
Cu1—O3	1.9408 (15)	C6—C7	1.369 (3)
Cu1—N2	1.9670 (19)	C6—H6	0.9300
Cu1—N1	2.032 (2)	C7—C8	1.390 (4)
N1—C3	1.279 (3)	C7—H7	0.9300
N1—O1	1.415 (3)	C8—C9	1.372 (4)
N2—C11	1.289 (3)	C9—H9	0.9300
N2—O2	1.432 (2)	C10—H10A	0.9600
O1—C1	1.425 (3)	C10—H10B	0.9600
O2—C2	1.435 (3)	C10—H10C	0.9600
O3—C5	1.319 (3)	C11—C12	1.423 (4)
O4—C8	1.379 (3)	C11—H11	0.9300
O4—C10	1.412 (4)	C12—C13	1.415 (3)
O5—C13	1.308 (3)	C12—C17	1.419 (4)
O6—C16	1.388 (3)	C13—C14	1.410 (3)
O6—C18	1.406 (4)	C14—C15	1.367 (4)
C1—C2	1.500 (3)	C14—H14	0.9300
C1—H1A	0.9700	C15—C16	1.395 (4)
C1—H1B	0.9700	C15—H15	0.9300
C2—H2A	0.9700	C16—C17	1.363 (4)
C2—H2B	0.9700	C17—H17	0.9300
C3—C4	1.438 (3)	C18—H18A	0.9600
C3—H3	0.9300	C18—H18B	0.9600
C4—C5	1.410 (3)	C18—H18C	0.9600
C4—C9	1.413 (4)		
O5—Cu1—O3	87.53 (7)	C6—C7—C8	120.9 (2)
O5—Cu1—N2	89.62 (8)	C6—C7—H7	119.5
O3—Cu1—N2	164.87 (8)	C8—C7—H7	119.5
O5—Cu1—N1	173.80 (8)	C9—C8—O4	125.6 (2)
O3—Cu1—N1	87.50 (7)	C9—C8—C7	119.0 (2)
N2—Cu1—N1	94.22 (8)	O4—C8—C7	115.4 (2)
C3—N1—O1	109.3 (2)	C8—C9—C4	120.5 (2)
C3—N1—Cu1	123.67 (17)	C8—C9—H9	119.7
O1—N1—Cu1	126.72 (15)	C4—C9—H9	119.7
C11—N2—O2	110.71 (18)	O4—C10—H10A	109.5
C11—N2—Cu1	128.51 (17)	O4—C10—H10B	109.5

O2—N2—Cu1	119.63 (14)	H10A—C10—H10B	109.5
N1—O1—C1	112.32 (18)	O4—C10—H10C	109.5
N2—O2—C2	109.72 (16)	H10A—C10—H10C	109.5
C5—O3—Cu1	123.45 (14)	H10B—C10—H10C	109.5
C8—O4—C10	117.5 (2)	N2—C11—C12	125.0 (2)
C13—O5—Cu1	130.08 (15)	N2—C11—H11	117.5
C16—O6—C18	117.0 (2)	C12—C11—H11	117.5
O1—C1—C2	110.4 (2)	C13—C12—C17	120.1 (2)
O1—C1—H1A	109.6	C13—C12—C11	121.5 (2)
C2—C1—H1A	109.6	C17—C12—C11	118.3 (2)
O1—C1—H1B	109.6	O5—C13—C14	118.8 (2)
C2—C1—H1B	109.6	O5—C13—C12	124.4 (2)
H1A—C1—H1B	108.1	C14—C13—C12	116.8 (2)
O2—C2—C1	113.3 (2)	C15—C14—C13	122.3 (2)
O2—C2—H2A	108.9	C15—C14—H14	118.9
C1—C2—H2A	108.9	C13—C14—H14	118.9
O2—C2—H2B	108.9	C14—C15—C16	120.5 (3)
C1—C2—H2B	108.9	C14—C15—H15	119.8
H2A—C2—H2B	107.7	C16—C15—H15	119.8
N1—C3—C4	125.3 (2)	C17—C16—O6	125.8 (3)
N1—C3—H3	117.3	C17—C16—C15	119.6 (2)
C4—C3—H3	117.3	O6—C16—C15	114.5 (3)
C5—C4—C9	121.1 (2)	C16—C17—C12	120.7 (2)
C5—C4—C3	121.2 (2)	C16—C17—H17	119.6
C9—C4—C3	117.6 (2)	C12—C17—H17	119.6
O3—C5—C6	119.6 (2)	O6—C18—H18A	109.5
O3—C5—C4	124.3 (2)	O6—C18—H18B	109.5
C6—C5—C4	116.0 (2)	H18A—C18—H18B	109.5
C7—C6—C5	122.4 (2)	O6—C18—H18C	109.5
C7—C6—H6	118.8	H18A—C18—H18C	109.5
C5—C6—H6	118.8	H18B—C18—H18C	109.5
O5—Cu1—N1—C3	−5.1 (8)	C3—C4—C5—C6	−174.8 (2)
O3—Cu1—N1—C3	31.6 (2)	O3—C5—C6—C7	178.9 (2)
N2—Cu1—N1—C3	−133.3 (2)	C4—C5—C6—C7	−1.6 (4)
O5—Cu1—N1—O1	168.3 (6)	C5—C6—C7—C8	−0.2 (4)
O3—Cu1—N1—O1	−154.89 (18)	C10—O4—C8—C9	0.0 (4)
N2—Cu1—N1—O1	40.17 (19)	C10—O4—C8—C7	179.7 (3)
O5—Cu1—N2—C11	1.3 (2)	C6—C7—C8—C9	1.7 (4)
O3—Cu1—N2—C11	80.4 (4)	C6—C7—C8—O4	−178.0 (2)
N1—Cu1—N2—C11	176.4 (2)	O4—C8—C9—C4	178.3 (2)
O5—Cu1—N2—O2	−165.28 (15)	C7—C8—C9—C4	−1.4 (4)
O3—Cu1—N2—O2	−86.2 (3)	C5—C4—C9—C8	−0.4 (4)
N1—Cu1—N2—O2	9.85 (16)	C3—C4—C9—C8	176.4 (2)
C3—N1—O1—C1	−177.0 (2)	O2—N2—C11—C12	173.7 (2)
Cu1—N1—O1—C1	8.8 (3)	Cu1—N2—C11—C12	6.2 (4)
C11—N2—O2—C2	106.1 (2)	N2—C11—C12—C13	−8.2 (4)
Cu1—N2—O2—C2	−85.07 (19)	N2—C11—C12—C17	173.5 (2)
O5—Cu1—O3—C5	136.42 (18)	Cu1—O5—C13—C14	−172.55 (17)
N2—Cu1—O3—C5	57.1 (4)	Cu1—O5—C13—C12	9.2 (4)

N1—Cu1—O3—C5	−39.87 (18)	C17—C12—C13—O5	178.7 (2)
O3—Cu1—O5—C13	−174.0 (2)	C11—C12—C13—O5	0.4 (4)
N2—Cu1—O5—C13	−8.9 (2)	C17—C12—C13—C14	0.4 (4)
N1—Cu1—O5—C13	−137.2 (6)	C11—C12—C13—C14	−177.9 (2)
N1—O1—C1—C2	−89.8 (2)	O5—C13—C14—C15	−178.0 (2)
N2—O2—C2—C1	60.0 (3)	C12—C13—C14—C15	0.3 (4)
O1—C1—C2—O2	51.2 (3)	C13—C14—C15—C16	−1.4 (4)
O1—N1—C3—C4	173.7 (2)	C18—O6—C16—C17	−1.3 (5)
Cu1—N1—C3—C4	−11.9 (4)	C18—O6—C16—C15	177.7 (3)
N1—C3—C4—C5	−13.5 (4)	C14—C15—C16—C17	1.6 (4)
N1—C3—C4—C9	169.8 (2)	C14—C15—C16—O6	−177.4 (3)
Cu1—O3—C5—C6	−151.11 (17)	O6—C16—C17—C12	178.1 (3)
Cu1—O3—C5—C4	29.4 (3)	C15—C16—C17—C12	−0.8 (4)
C9—C4—C5—O3	−178.7 (2)	C13—C12—C17—C16	−0.2 (4)
C3—C4—C5—O3	4.7 (4)	C11—C12—C17—C16	178.2 (3)
C9—C4—C5—C6	1.8 (3)		

Fig. 1

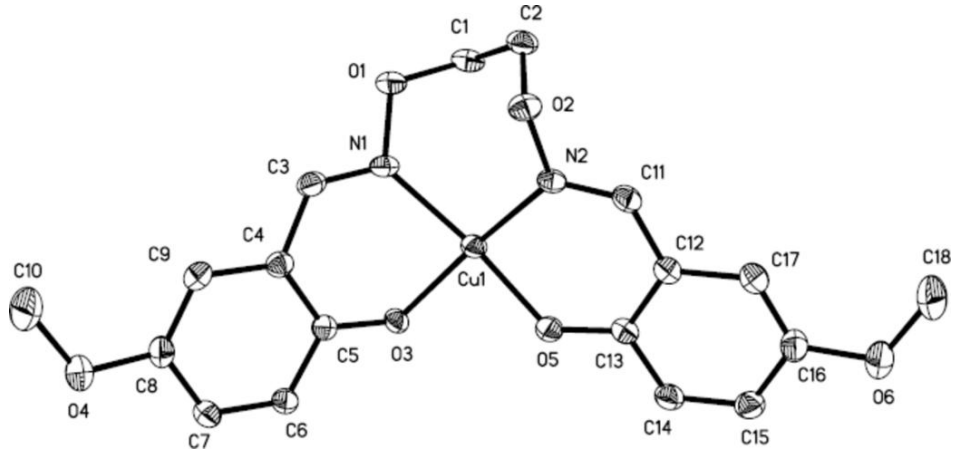

C1
C2
O1
O2
N1
N2
C3
C11
C4
C12
C9
C17
C18
C10
Cu1
C5
O3
O5
C13
C16
O6
C8
O4
C7
C6
C14
C15

Fig. 2