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[*N*,*N*′-Bis(6-methoxysalicylidene)-1,3-diaminopropane]copper(II)

Mohammad Hossein Habibi,[a]* Reza Mokhtari,[a] Ross W. Harrington[b] and William Clegg[b]

[a]Center of Excellence (Catalysis and Fuel Cells), Department of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran, and [b]School of Natural Sciences (Chemistry), Newcastle University, Newcastle Upon Tyne NE1 7RU, England
Correspondence e-mail: habibi@chem.ui.ac.ir

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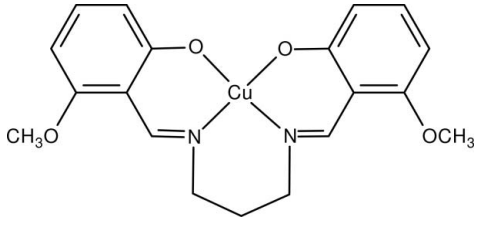
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.063; data-to-parameter ratio = 17.5.

The title compound, [Cu($C_{19}H_{20}N_2O_4$)], is a mononuclear copper(II) Schiff base complex. The Cu^{II} ion is surrounded by two imine N and two phenolate O atoms of the tetradentate ligand in a square-planar coordination with a slight tetrahedral distortion. The dihedral angle between the CuN_2 and CuO_2 planes is 25.07 (9)°.

Related literature

A review of ligand environments and structures of Schiff base adducts and tetracoordinated metal chelates has been given by Garnovskii *et al.* (1993). The Cambridge Structural Database (Version 5.28, plus two updates, May 2007; Allen, 2002) was used as a source for searching for related structures. For comparable Schiff base complexes, see: Elerman *et al.* (1991); Nathan *et al.* (2003).



Experimental

Crystal data

[Cu($C_{19}H_{20}N_2O_4$)]
M_r = 403.91
Orthorhombic, $Pca2_1$
a = 13.7911 (14) Å
b = 12.7032 (13) Å
c = 9.9329 (10) Å
V = 1740.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 150 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005*a*)
T_{min} = 0.700, T_{max} = 0.785
14731 measured reflections
4157 independent reflections
3766 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.04
4157 reflections
237 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), with 1916 Friedel pairs
Flack parameter: 0.013 (12)

Table 1
Selected geometric parameters (Å, °).

Cu—N1	1.9554 (15)	Cu—O2	1.9136 (14)
Cu—N2	1.9602 (15)	Cu—O3	1.8996 (13)
N1—Cu—N2	96.88 (6)	N2—Cu—O2	163.48 (6)
N1—Cu—O2	91.31 (6)	N2—Cu—O3	92.48 (6)
N1—Cu—O3	159.21 (6)	O2—Cu—O3	84.63 (6)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2129).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Brandenburg, K. (2007). *DIAMOND*. Version 3.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Elerman, Y., Svoboda, I. & Fuess, H. (1991). *Z. Kristallogr.* **196**, 309–311.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Nathan, L. C., Koehne, J. E., Gilmore, J. M., Hannibal, K. A., Dewhirst, W. E. & Mai, T. D. (2003). *Polyhedron*, **22**, 887–894.
Sheldrick, G. M. (2005*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2005*b*). *SHELXTL*. Version 6. Bruker AXS Inc., Madison, Wisconsin, USA.

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supplementary materials

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[*N*,*N*'-Bis(6-methoxysalicylidene)-1,3-diaminopropane]copper(II)

M. H. Habibi, R. Mokhtari, R. W. Harrington and W. Clegg

Comment

Metal derivatives of Schiff bases have been studied extensively, and Cu^{II} and Ni^{II} complexes play a major role in both synthetic and structural research. The coordination of the metal cations is usually planar in the case of Ni, but for Cu a tetrahedral distortion is often observed (Garnovskii *et al.*, 1993). We report here the results of the reaction of Cu^{II} with the tetradentate ligand *N*,*N*'-bis(6-methoxysalicylidene)-1,3-diaminopropane in a 1:1 molar ratio, forming the title compound, (I).

A view of the molecular structure of (I) is shown in Fig. 1. The crystal structure of the ligand (but without methoxy substituents) is known for a long time (Elerman *et al.*, 1991), as are about 150 of its metal complexes (found in a search of the Cambridge Structural Database [version 5.28] plus two updates until May 2007; Allen, 2002). Structures of the Cu^{II} complex which are comparable with the title compound have been reported several times, the most recent given by Nathan *et al.* (2003). The title complex, however, is the first reported example of a Schiff base, as a ligand or uncomplexed, in which substituents in the 6 position of the benzene rings are present.

The Cu^{II} coordination polyhedron is approximately square planar, with a significant distortion towards tetrahedral, as indicated by the dihedral angle of 25.07 (9)° between the CuO_2 and CuN_2 planes. This, and the Cu—O and Cu—N distances (see Table), are similar to those observed in other Cu^{II} complexes of related Schiff bases.

Experimental

A mixture of 6-methoxysalicylaldehyde (2.0 mmol, 304 mg) and 1,3-diaminopropane (1.0 mmol, 74 mg) was dissolved in methanol (10 ml) with stirring for 30 min at room temperature, to give a clear yellow solution. A methanol solution (10 ml) of $Cu(CH_3COO)_2{\cdot}2H_2O$ (1.0 mmol, 218 mg) was then added. The mixture was stirred for further 30 min and then filtered. After keeping the filtrate in air for 7 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent, in about 65% yield.

Refinement

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Figures

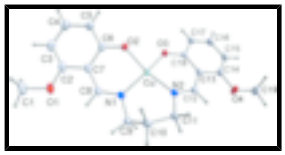

Fig. 1. The molecular structure with atom labels, drawn with ellipsoids at the 50% probability level for all non-H atoms. H atoms are given as spheres of arbitrary radius.

{2,2'-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}copper(II)

Crystal data

$[Cu(C_{19}H_{20}N_2O_4)]$	$F_{000} = 836$
$M_r = 403.91$	$D_x = 1.542$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2ac	Cell parameters from 9351 reflections
$a = 13.7911$ (14) Å	$\theta = 2.2$–$28.3°$
$b = 12.7032$ (13) Å	$\mu = 1.28$ mm^{-1}
$c = 9.9329$ (10) Å	$T = 150$ (2) K
$V = 1740.2$ (3) Å^3	Block, blue
$Z = 4$	0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer	4157 independent reflections
Radiation source: fine-focus sealed tube	3766 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 150(2)$ K	$\theta_{max} = 28.3°$
ω scans	$\theta_{min} = 2.2°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2005a)	$h = -17 \rightarrow 17$
$T_{min} = 0.700$, $T_{max} = 0.785$	$k = -16 \rightarrow 16$
14731 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 0.2389P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.063$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
4157 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
237 parameters	Extinction correction: none

1 restraint	Absolute structure: Flack (1983), 1916 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.013 (12)
Secondary atom site location: difference Fourier map	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu	0.174992 (13)	0.252482 (15)	0.36441 (5)	0.01625 (6)
N1	0.23946 (12)	0.12304 (12)	0.42218 (15)	0.0194 (3)
N2	0.28978 (10)	0.32088 (11)	0.28765 (16)	0.0171 (3)
O1	0.13783 (12)	−0.12408 (11)	0.62238 (16)	0.0321 (3)
O2	0.06371 (10)	0.22063 (11)	0.47204 (15)	0.0239 (3)
O3	0.08904 (9)	0.34212 (10)	0.26854 (13)	0.0210 (3)
O4	0.30881 (10)	0.53932 (12)	0.00073 (16)	0.0298 (3)
C1	0.1202 (2)	−0.20841 (18)	0.7155 (3)	0.0402 (6)
H1A	0.1723	−0.2605	0.7085	0.060*
H1B	0.0580	−0.2419	0.6942	0.060*
H1C	0.1181	−0.1803	0.8074	0.060*
C2	0.07334 (16)	−0.04266 (15)	0.6220 (2)	0.0244 (4)
C3	−0.01325 (16)	−0.04319 (16)	0.6918 (2)	0.0284 (5)
H3A	−0.0321	−0.1025	0.7438	0.034*
C4	−0.07236 (16)	0.04570 (17)	0.6838 (2)	0.0292 (4)
H4A	−0.1319	0.0460	0.7320	0.035*
C5	−0.04815 (15)	0.13287 (16)	0.6092 (2)	0.0258 (4)
H5A	−0.0913	0.1911	0.6052	0.031*
C6	0.04105 (14)	0.13626 (15)	0.53826 (18)	0.0208 (4)
C7	0.10334 (15)	0.04696 (15)	0.54488 (19)	0.0205 (4)
C8	0.19971 (14)	0.04821 (15)	0.49065 (19)	0.0210 (4)
H8A	0.2384	−0.0124	0.5068	0.025*
C9	0.34254 (14)	0.11051 (14)	0.38763 (19)	0.0221 (4)
H9A	0.3495	0.1006	0.2892	0.027*
H9B	0.3691	0.0475	0.4332	0.027*
C10	0.39877 (15)	0.20812 (16)	0.4319 (2)	0.0227 (4)
H10A	0.3736	0.2323	0.5199	0.027*
H10B	0.4679	0.1893	0.4439	0.027*
C11	0.39108 (13)	0.29754 (15)	0.33088 (19)	0.0207 (4)
H11A	0.4194	0.3618	0.3712	0.025*
H11B	0.4300	0.2795	0.2504	0.025*
C12	0.28636 (14)	0.39154 (14)	0.19369 (18)	0.0182 (4)
H12A	0.3471	0.4145	0.1595	0.022*
C13	0.20214 (13)	0.43938 (14)	0.13492 (18)	0.0178 (4)

C14	0.21461 (13)	0.51992 (15)	0.03636 (19)	0.0204 (4)
C15	0.13649 (14)	0.57306 (15)	−0.0176 (2)	0.0226 (4)
H15A	0.1456	0.6263	−0.0835	0.027*
C16	0.04276 (14)	0.54632 (15)	0.0277 (2)	0.0241 (4)
H16A	−0.0116	0.5824	−0.0087	0.029*
C17	0.02793 (14)	0.46998 (15)	0.1223 (2)	0.0226 (4)
H17A	−0.0363	0.4541	0.1503	0.027*
C18	0.10671 (13)	0.41422 (14)	0.17916 (19)	0.0184 (4)
C19	0.32782 (15)	0.62249 (17)	−0.0922 (2)	0.0295 (5)
H19A	0.3979	0.6284	−0.1068	0.044*
H19B	0.3030	0.6889	−0.0556	0.044*
H19C	0.2956	0.6073	−0.1780	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.01746 (10)	0.01431 (10)	0.01697 (10)	0.00117 (8)	0.00155 (11)	0.00191 (8)
N1	0.0246 (8)	0.0166 (7)	0.0170 (7)	0.0037 (6)	0.0008 (6)	−0.0003 (6)
N2	0.0165 (7)	0.0159 (7)	0.0191 (8)	0.0017 (6)	−0.0019 (6)	−0.0002 (6)
O1	0.0434 (9)	0.0202 (7)	0.0328 (8)	−0.0012 (6)	0.0019 (7)	0.0100 (6)
O2	0.0252 (7)	0.0188 (6)	0.0278 (7)	0.0011 (6)	0.0083 (6)	0.0043 (6)
O3	0.0168 (6)	0.0202 (6)	0.0258 (7)	0.0017 (5)	0.0021 (5)	0.0066 (6)
O4	0.0179 (6)	0.0328 (8)	0.0388 (9)	−0.0034 (6)	0.0008 (6)	0.0191 (7)
C1	0.0548 (16)	0.0247 (11)	0.0412 (14)	−0.0029 (11)	−0.0002 (11)	0.0160 (10)
C2	0.0350 (11)	0.0190 (9)	0.0193 (9)	−0.0079 (8)	−0.0060 (8)	0.0005 (8)
C3	0.0362 (11)	0.0273 (10)	0.0217 (10)	−0.0148 (9)	−0.0026 (8)	0.0045 (8)
C4	0.0291 (11)	0.0356 (11)	0.0230 (10)	−0.0119 (9)	0.0008 (8)	0.0000 (9)
C5	0.0261 (10)	0.0278 (10)	0.0235 (10)	−0.0024 (8)	0.0026 (8)	0.0014 (8)
C6	0.0275 (10)	0.0203 (9)	0.0147 (8)	−0.0035 (7)	0.0006 (7)	−0.0008 (7)
C7	0.0296 (10)	0.0168 (9)	0.0151 (9)	−0.0037 (7)	−0.0018 (7)	0.0002 (7)
C8	0.0306 (10)	0.0152 (9)	0.0173 (9)	0.0007 (7)	−0.0023 (7)	−0.0020 (7)
C9	0.0247 (9)	0.0191 (8)	0.0224 (11)	0.0057 (7)	0.0033 (7)	0.0010 (7)
C10	0.0216 (9)	0.0236 (9)	0.0230 (10)	0.0053 (8)	−0.0035 (8)	0.0038 (8)
C11	0.0149 (9)	0.0222 (9)	0.0250 (11)	0.0016 (7)	−0.0033 (7)	0.0028 (7)
C12	0.0160 (8)	0.0181 (8)	0.0203 (9)	−0.0007 (7)	0.0001 (6)	−0.0002 (7)
C13	0.0177 (8)	0.0160 (8)	0.0196 (9)	0.0005 (7)	−0.0016 (7)	0.0023 (7)
C14	0.0174 (8)	0.0202 (9)	0.0236 (9)	−0.0020 (7)	−0.0003 (7)	0.0031 (7)
C15	0.0244 (9)	0.0183 (9)	0.0252 (9)	0.0015 (7)	−0.0011 (8)	0.0062 (8)
C16	0.0215 (9)	0.0206 (10)	0.0301 (10)	0.0053 (7)	−0.0043 (8)	0.0038 (8)
C17	0.0162 (9)	0.0221 (9)	0.0295 (10)	0.0018 (7)	0.0019 (7)	0.0029 (8)
C18	0.0193 (9)	0.0160 (8)	0.0198 (9)	0.0005 (7)	0.0017 (7)	−0.0013 (7)
C19	0.0267 (10)	0.0298 (11)	0.0321 (11)	−0.0056 (8)	0.0026 (8)	0.0125 (9)

Geometric parameters (Å, °)

Cu—N1	1.9554 (15)	C6—C7	1.425 (3)
Cu—N2	1.9602 (15)	C7—C8	1.434 (3)
Cu—O2	1.9136 (14)	C8—H8A	0.950
Cu—O3	1.8996 (13)	C9—H9A	0.990

N1—C8	1.291 (2)	C9—H9B	0.990
N1—C9	1.471 (2)	C9—C10	1.527 (3)
N2—C11	1.491 (2)	C10—H10A	0.990
N2—C12	1.296 (2)	C10—H10B	0.990
O1—C1	1.436 (3)	C10—C11	1.519 (3)
O1—C2	1.364 (3)	C11—H11A	0.990
O2—C6	1.296 (2)	C11—H11B	0.990
O3—C18	1.299 (2)	C12—H12A	0.950
O4—C14	1.369 (2)	C12—C13	1.435 (3)
O4—C19	1.427 (2)	C13—C14	1.426 (2)
C1—H1A	0.980	C13—C18	1.424 (3)
C1—H1B	0.980	C14—C15	1.380 (3)
C1—H1C	0.980	C15—H15A	0.950
C2—C3	1.381 (3)	C15—C16	1.410 (3)
C2—C7	1.433 (3)	C16—H16A	0.950
C3—H3A	0.950	C16—C17	1.366 (3)
C3—C4	1.395 (3)	C17—H17A	0.950
C4—H4A	0.950	C17—C18	1.415 (3)
C4—C5	1.373 (3)	C19—H19A	0.980
C5—H5A	0.950	C19—H19B	0.980
C5—C6	1.419 (3)	C19—H19C	0.980
N1—Cu—N2	96.88 (6)	N1—C9—H9B	109.7
N1—Cu—O2	91.31 (6)	N1—C9—C10	109.62 (15)
N1—Cu—O3	159.21 (6)	H9A—C9—H9B	108.2
N2—Cu—O2	163.48 (6)	H9A—C9—C10	109.7
N2—Cu—O3	92.48 (6)	H9B—C9—C10	109.7
O2—Cu—O3	84.63 (6)	C9—C10—H10A	109.1
Cu—N1—C8	125.50 (14)	C9—C10—H10B	109.1
Cu—N1—C9	117.51 (11)	C9—C10—C11	112.44 (17)
C8—N1—C9	116.98 (16)	H10A—C10—H10B	107.8
Cu—N2—C11	123.81 (12)	H10A—C10—C11	109.1
Cu—N2—C12	123.91 (13)	H10B—C10—C11	109.1
C11—N2—C12	112.28 (15)	N2—C11—C10	113.84 (16)
C1—O1—C2	117.18 (19)	N2—C11—H11A	108.8
Cu—O2—C6	130.69 (13)	N2—C11—H11B	108.8
Cu—O3—C18	130.41 (12)	C10—C11—H11A	108.8
C14—O4—C19	118.35 (15)	C10—C11—H11B	108.8
O1—C1—H1A	109.5	H11A—C11—H11B	107.7
O1—C1—H1B	109.5	N2—C12—H12A	116.0
O1—C1—H1C	109.5	N2—C12—C13	128.01 (18)
H1A—C1—H1B	109.5	H12A—C12—C13	116.0
H1A—C1—H1C	109.5	C12—C13—C14	119.04 (16)
H1B—C1—H1C	109.5	C12—C13—C18	121.84 (17)
O1—C2—C3	123.98 (18)	C14—C13—C18	118.96 (16)
O1—C2—C7	114.55 (19)	O4—C14—C13	114.90 (16)
C3—C2—C7	121.5 (2)	O4—C14—C15	123.54 (17)
C2—C3—H3A	120.9	C13—C14—C15	121.56 (17)
C2—C3—C4	118.23 (19)	C14—C15—H15A	120.8
H3A—C3—C4	120.9	C14—C15—C16	118.30 (18)

C3—C4—H4A	118.6	H15A—C15—C16	120.8
C3—C4—C5	122.8 (2)	C15—C16—H16A	119.1
H4A—C4—C5	118.6	C15—C16—C17	121.85 (17)
C4—C5—H5A	119.9	H16A—C16—C17	119.1
C4—C5—C6	120.22 (19)	C16—C17—H17A	119.5
H5A—C5—C6	119.9	C16—C17—C18	121.01 (17)
O2—C6—C5	119.12 (18)	H17A—C17—C18	119.5
O2—C6—C7	122.45 (17)	O3—C18—C13	122.87 (16)
C5—C6—C7	118.42 (18)	O3—C18—C17	118.81 (16)
C2—C7—C6	118.89 (18)	C13—C18—C17	118.31 (17)
C2—C7—C8	118.50 (18)	O4—C19—H19A	109.5
C6—C7—C8	122.19 (17)	O4—C19—H19B	109.5
N1—C8—C7	126.84 (18)	O4—C19—H19C	109.5
N1—C8—H8A	116.6	H19A—C19—H19B	109.5
C7—C8—H8A	116.6	H19A—C19—H19C	109.5
N1—C9—H9A	109.7	H19B—C19—H19C	109.5
N2—Cu—N1—C8	174.63 (16)	C3—C2—C7—C6	−1.4 (3)
N2—Cu—N1—C9	−3.89 (14)	C3—C2—C7—C8	171.33 (19)
O2—Cu—N1—C8	9.01 (16)	Cu—N1—C8—C7	−4.0 (3)
O2—Cu—N1—C9	−169.52 (13)	C9—N1—C8—C7	174.53 (18)
O3—Cu—N1—C8	−69.2 (3)	C2—C7—C8—N1	−178.13 (18)
O3—Cu—N1—C9	112.24 (19)	C6—C7—C8—N1	−5.7 (3)
N1—Cu—N2—C11	−25.55 (15)	Cu—N1—C9—C10	51.28 (18)
N1—Cu—N2—C12	154.49 (15)	C8—N1—C9—C10	−127.38 (18)
O2—Cu—N2—C11	93.6 (3)	N1—C9—C10—C11	−81.9 (2)
O2—Cu—N2—C12	−86.3 (3)	Cu—N2—C11—C10	5.3 (2)
O3—Cu—N2—C11	173.05 (14)	C12—N2—C11—C10	−174.79 (16)
O3—Cu—N2—C12	−6.91 (15)	C9—C10—C11—N2	49.3 (2)
N1—Cu—O2—C6	−8.50 (17)	Cu—N2—C12—C13	5.1 (3)
N2—Cu—O2—C6	−128.4 (2)	C11—N2—C12—C13	−174.83 (18)
O3—Cu—O2—C6	151.08 (17)	N2—C12—C13—C14	176.99 (18)
N1—Cu—O3—C18	−112.2 (2)	N2—C12—C13—C18	1.7 (3)
N2—Cu—O3—C18	4.62 (16)	C19—O4—C14—C13	−176.82 (17)
O2—Cu—O3—C18	168.31 (16)	C19—O4—C14—C15	3.2 (3)
C1—O1—C2—C3	−8.9 (3)	C12—C13—C14—O4	4.0 (3)
C1—O1—C2—C7	169.63 (19)	C12—C13—C14—C15	−176.04 (18)
O1—C2—C3—C4	179.44 (19)	C18—C13—C14—O4	179.49 (17)
C7—C2—C3—C4	1.0 (3)	C18—C13—C14—C15	−0.6 (3)
C2—C3—C4—C5	0.4 (3)	O4—C14—C15—C16	−179.7 (2)
C3—C4—C5—C6	−1.3 (3)	C13—C14—C15—C16	0.3 (3)
Cu—O2—C6—C5	−179.00 (14)	C14—C15—C16—C17	−0.1 (3)
Cu—O2—C6—C7	2.3 (3)	C15—C16—C17—C18	0.0 (3)
C4—C5—C6—O2	−177.84 (19)	Cu—O3—C18—C13	0.2 (3)
C4—C5—C6—C7	0.9 (3)	Cu—O3—C18—C17	179.72 (13)
O2—C6—C7—C2	179.10 (17)	C16—C17—C18—O3	−179.84 (18)
O2—C6—C7—C8	6.7 (3)	C16—C17—C18—C13	−0.3 (3)
C5—C6—C7—C2	0.4 (3)	C12—C13—C18—O3	−4.6 (3)
C5—C6—C7—C8	−172.05 (18)	C12—C13—C18—C17	175.85 (18)
O1—C2—C7—C6	−179.93 (17)	C14—C13—C18—O3	−179.93 (17)

O1—C2—C7—C8	−7.2 (3)	C14—C13—C18—C17	0.5 (3)

Fig. 1