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Dichlorido-1κCl,3κCl-bis{μ-2,2′-[propane-1,3-diylbis(iminomethylene)]diphenolato}-1:2$\kappa^6O,N,N',O':O,O'$;2:3$\kappa^6O,O':O,N,N',O'$-tricopper(II)

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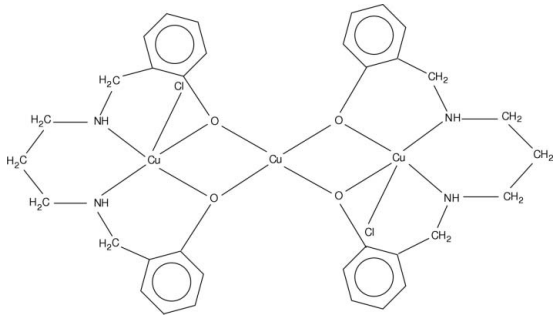
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.076; data-to-parameter ratio = 15.8.

The title linear trinuclear copper(II) complex, $[Cu_3(C_{17}H_{20}N_2O_2)_2Cl_2]$, was obtained from *N*,*N*′-bis(2-hydroxybenzyl)-1,3-propanediamine and $CuCl_2$. The overall charge of the three Cu^{2+} ions is balanced by four deprotonated phenol groups and two Cl^- ligands. The complex is centrosymmetric with the central Cu^{2+} occupying a special position ($\bar{1}$). This Cu^{2+} ion is coordinated by the four phenolate O atoms in a square-planar fashion. The second Cu^{2+} occupies a general position in a square-pyramidal fashion. Two phenolate O atoms and two amine N form the basal plane, with Cl^- ligands occupying the fifth coordination site.

Related literature

For related literature, see: Addison *et al.* (1984); Atakol *et al.* (1999); Cremer & Pople (1975); Ercan *et al.* (2002); Fukuhara *et al.* (1990); Gerli *et al.* (1991); Mikuriya *et al.* (2001); Song *et al.* (2003, 2005); Spek (2003); Uhlenbrock *et al.* (1996); Yıldırım & Atakol (2002).



Experimental

Crystal data

$[Cu_3(C_{17}H_{20}N_2O_2)_2Cl_2]$
M_r = 830.25
Monoclinic, $P2_1/c$
a = 11.0189 (7) Å
b = 15.3861 (8) Å
c = 10.7441 (8) Å
β = 106.959 (7)°
V = 1742.3 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.01 mm^{-1}
T = 100 (2) K
0.36 × 0.22 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min} = 0.531, T_{max} = 0.766
12067 measured reflections
3481 independent reflections
2969 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.10
3481 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu2—Cl1	2.5092 (7)	O2—Cu1	1.9108 (16)
Cu2—Cu1	2.9138 (3)	O2—Cu2	1.9632 (16)
O1—Cu1	1.9191 (15)	N1—Cu2	1.995 (2)
O1—Cu2	1.9825 (16)	N2—Cu2	1.995 (2)
O2—Cu1—O1	80.93 (7)	O2—Cu2—N2	93.17 (7)
O2—Cu1—Cu2	41.91 (5)	O1—Cu2—N2	168.74 (8)
O1—Cu1—Cu2	42.52 (5)	O2—Cu2—Cl1	89.92 (5)
O2—Cu2—O1	78.09 (7)	O1—Cu2—Cl1	88.09 (5)
O2—Cu2—N1	163.99 (8)	Cu1—O1—Cu2	96.62 (7)
O1—Cu2—N1	92.91 (7)	Cu1—O2—Cu2	97.54 (7)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2056).

References

Addison, A. W., Rao, T. N., Reedijk, J., Van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
Atakol, O., Arıcı, C., Ercan, F. & Ülkü, D. (1999). *Acta Cryst.* C**55**, 511–513.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Ercan, F., Atakol, O., Arıcı, C., Svoboda, I. & Fuess, H. (2002). *Acta Cryst.* C**58**, m193–m196.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

 doi:10.1107/S1600536808003048

Fukuhara, C., Tsuneyoshi, K., Matsumoto, N., Kida, S., Mikuriya, M. & Mori, M. (1990). *J. Chem. Soc. Dalton Trans.* pp. 3473–3479.
Gerli, A., Hagen, K. S. & Marzilli, L. G. (1991). *Inorg. Chem.* **30**, 4673–4676.
Mikuriya, M., Ikenove, S., Nukada, R. & Lim, J. W. (2001). *Bull. Chem. Soc. Jpn*, **74**, 101–102.
Oxford Diffraction (2002). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd., Poland.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, Y., Gomez, P., Roubeav, O., Lutz, M., Spek, A. L. & Reedijk, J. (2003). *Eur. J. Inorg. Chem.* pp. 2924–2928.
Song, Y., Gomez, P., Roubeav, O., Mutikainen, I., Turpeinen, U. & Reedijk, J. (2005). *Inorg. Chim. Acta*, **358**, 109–115.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Uhlenbrock, S., Wegner, R. & Krebs, B. (1996). *J. Chem. Soc. Dalton Trans.* pp. 3731–3736.
Yıldırım, L. T. & Atakol, O. (2002). *Cryst. Res. Technol.* **37**, 1352–1359.

supporting information

Acta Cryst. (2008). E**64**, m481–m482 [doi:10.1107/S1600536808003048]

Dichlorido-1κCl,3κCl-bis{μ-2,2′-[propane-1,3-diylbis(iminomethylene)]diphenolato}-1:2$\kappa^6O,N,N',O':O,O'$;2:3$\kappa^6O,O':O,N,N',O'$-tricopper(II)

Bürke Meltem Ateş, Filiz Ercan, Ingrid Svoboda, Hartmut Fuess and Orhan Atakol

S1. Comment

Bis-*N*,*N*′-bis(2-hydroxybenzyl)-1,3-propane-diamine is an ONNO type Schiff base and there have been various polynuclear complexes synthesized since 1990 (Fukuhara *et al.*, 1990; Gerli *et al.*, 1991; Uhlenbrock *et al.*, 1996, Mikuriya *et al.*, 2001).

In this study, *N*,*N*′-bis(salicylidene)-1,3-propane-diamine was reduced into a symmetrical phenol-amine compound by the help of $NaBH_4$. A trinuclear Cu(II) complex was prepared by the reaction of the ligand obtained with $CuCl_2$ and its molecular structure was determined. Previously, this complex had been prepared in MeOH solution and crystallized in its tetra-solvated form (Song *et al.*, 2005). The trinuclear complex obtained in this structure is not solvated and has different crystallographic details.

As can seen from *PLATON* (Spek, 2003), the terminal Cu(II) ion has a square pyramidal coordination formed by the two phenolic oxygen and two iminic nitrogen atoms of the ligand and a chloride ion. There has been a T factor defined for five membered coordination sphere (Addison *et al.*, 1984). This factor is given as T=a-b/60, where a and b correspond to two largest angles around the metal atom. If T=0 the coordination is an ideal square pyramid and if T=1 the coordination is ideal trigonal bipyramid. If the values listed in molecular geometry are employed the T value is found as 0.078 indicating that the terminal Cu(II) atoms has a near ideal square pyramidal symmetry. The Cu—Cl bond is longer than other coordination bonds (2.509 Å). The bond length in the square base are very close to each other (1.963 Å). The chalate ring (Cu2, N1, N2, C8, C9, C10) formed by the terminal Cu(II) ions has an almost ideal chair conformation. The conformation of the ring was analysed using *PLATON*. The Cremer-Pople puckering parameters are Q_T=1.374 (6), θ=-38.9 (2), φ=120.34 (12)° (Cremer *et al.*, 1975).

The central Cu(II) ion is coordinated between four phenolic oxygen donors. The Cu1—O2 and Cu1—O1 distances are 1.911 Å and 1.919 Å, respectively. The phenolic O atoms act as bridging ligands between the central and the terminal Cu ions. The distance between Cu2 and an L.S. plane through O1, N1, N2 and O2 is 0.1894 (3) Å.. That is why the six membered chelate ring conformation of Schiff base complexes was reported as almost ideal (Yıldırım *et al.*, 2002). The smallest Cu—Cu distance determined in similar complexes was reported as 2.914 Å (Song *et al.*, 2005; Song *et al.*, 2003). The Cu2—Cu1 distance in the title compound is 2.9138 (3) Å and thus close to the shortest reported distances. In complexes containing *m*-bonds such as AcO– and HCOO– this distance is bigger than 3.0 Å (Ercan *et al.*, 2002; Atakol *et al.*, 1999).

S2. Experimental

N,*N*′-bis(salicylidene)-1,3-propane-diamine was dissolved by slightly heating in MeOH (80 ml). $NaBH_4$ was added into this solution in its solid form with small portions and the resulting mixture was rigorously stirred. The addition of $NaBH_4$ was continued unless the solution became completely colorless. The colorless solution was mixed with ice (300 g) and

kept on the bench for 24 h. The white precipitate was the reduced product of *N*,*N*′-bis(2-hydroxybenzyl)-1,3-propane-diamine (m.p. 379–380 K, yield % 87, the N—H streching band is observed at 3273 cm^{-1}). *N*,*N*′-bis (2-hydroxybenzyl)-1,3-propane-diamine (0.285 g, 1 mmole) was dissolved in dmf (dimethyl-formamide)(20 ml) by heating and a solution of $CuCl_2.2H_2O$ (0.255 g, 1.5 mmole) in hot dmf (20 ml) was added to it and the resulting mixture was kept on the bench for 4–5 d. The resulting crystals were filtered off, washed with EtOH and dried in oven at 353 K.

S3. Refinement

H1A and H2A (for NH) were located in a Fourier map and only their positions refined [N—H = 0.82 (3) and 0.86 (3) Å, U_{iso}(H) = 0.028 and 0.028 $Å^2$]. The remaining H atoms were positioned geometrically, with C—H = 0.95 and 0.99 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

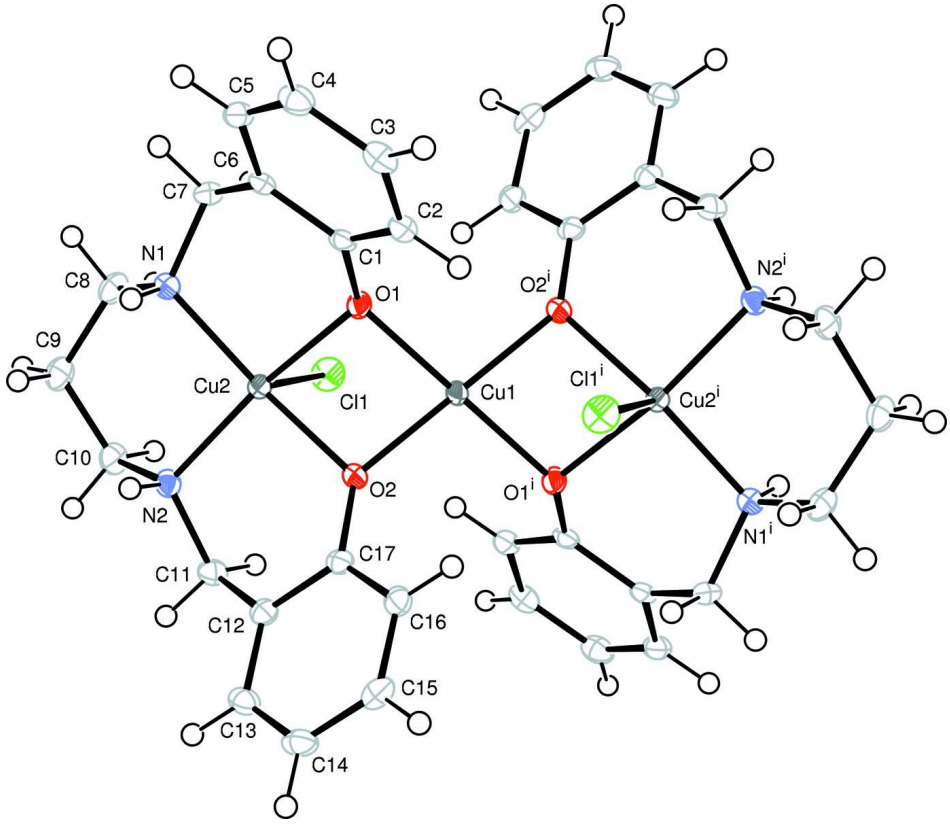

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (i) -*x*, -*y*, 1 - *z*].

Dichlorido-1κCl,3κCl-bis{μ-2,2′-[propane-1,3- diylbis(iminomethylene)]diphenolato}-1:2$\kappa^6 O,N,N',O'$:O,O';2:3$\kappa^6 O,O'$:O,N,N',O'-tricopper(II)

Crystal data

$[Cu_3(C_{17}H_{20}N_2O_2)_2Cl_2]$
M_r = 830.25
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.0189 (7) Å
b = 15.3861 (8) Å
c = 10.7441 (8) Å
β = 106.959 (7)°
V = 1742.3 (2) $Å^3$
Z = 2
F(000) = 850
D_x = 1.583 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4076 reflections
θ = 2.4–26.4°
μ = 2.01 mm^{-1}
T = 100 K
Prism, dark green
0.36 × 0.22 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min} = 0.531, T_{max} = 0.766
12067 measured reflections
3481 independent reflections
2969 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.4°, θ_{min} = 4.1°
h = −13→13
k = −18→18
l = −7→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.10
3481 reflections
220 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
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
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 1.1376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.019
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.0000	0.0000	0.5000	0.01443 (11)
Cu2	0.02986 (3)	0.187585 (17)	0.48593 (3)	0.01380 (10)
Cl1	0.04255 (6)	0.16106 (4)	0.71982 (6)	0.02363 (16)
O1	−0.10643 (15)	0.09894 (10)	0.43769 (17)	0.0170 (4)
O2	0.12675 (15)	0.08066 (10)	0.48475 (17)	0.0187 (4)
N1	−0.09257 (18)	0.28603 (13)	0.4363 (2)	0.0153 (4)
H1A	−0.080 (3)	0.3050 (19)	0.369 (3)	0.028*
N2	0.18192 (18)	0.26353 (13)	0.5115 (2)	0.0158 (4)
H2A	0.180 (3)	0.2855 (19)	0.437 (3)	0.028*
C1	−0.2034 (2)	0.10818 (15)	0.3275 (2)	0.0153 (5)
C2	−0.2429 (2)	0.04128 (16)	0.2376 (2)	0.0185 (5)
H2	−0.2027	−0.0139	0.2531	0.022*

C3	−0.3414 (2)	0.05583 (17)	0.1253 (3)	0.0214 (5)
H3	−0.3684	0.0102	0.0639	0.026*
C4	−0.4010 (2)	0.13600 (17)	0.1012 (3)	0.0222 (6)
H4	−0.4680	0.1455	0.0236	0.027*
C5	−0.3617 (2)	0.20233 (16)	0.1919 (2)	0.0198 (5)
H5	−0.4021	0.2574	0.1753	0.024*
C6	−0.2644 (2)	0.18960 (15)	0.3063 (2)	0.0159 (5)
C7	−0.2269 (2)	0.25755 (16)	0.4097 (2)	0.0188 (5)
H7A	−0.2831	0.3086	0.3828	0.023*
H7B	−0.2396	0.2344	0.4910	0.023*
C8	−0.0623 (2)	0.35758 (15)	0.5329 (3)	0.0202 (5)
H8A	−0.0640	0.3349	0.6186	0.024*
H8B	−0.1282	0.4031	0.5063	0.024*
C9	0.0669 (2)	0.39773 (15)	0.5461 (3)	0.0216 (6)
H9A	0.0678	0.4190	0.4594	0.026*
H9B	0.0771	0.4489	0.6041	0.026*
C10	0.1804 (2)	0.33853 (16)	0.5985 (3)	0.0208 (5)
H10A	0.2590	0.3728	0.6105	0.025*
H10B	0.1798	0.3163	0.6848	0.025*
C11	0.3017 (2)	0.21331 (16)	0.5631 (2)	0.0191 (5)
H11A	0.3026	0.1874	0.6477	0.023*
H11B	0.3744	0.2539	0.5792	0.023*
C12	0.3198 (2)	0.14203 (15)	0.4743 (2)	0.0160 (5)
C13	0.4258 (2)	0.13781 (16)	0.4284 (2)	0.0198 (5)
H13	0.4855	0.1840	0.4470	0.024*
C14	0.4451 (2)	0.06791 (17)	0.3567 (3)	0.0226 (6)
H14	0.5182	0.0658	0.3268	0.027*
C15	0.3588 (2)	0.00111 (16)	0.3285 (2)	0.0205 (5)
H15	0.3731	−0.0473	0.2797	0.025*
C16	0.2508 (2)	0.00332 (15)	0.3702 (2)	0.0178 (5)
H16	0.1911	−0.0429	0.3494	0.021*
C17	0.2309 (2)	0.07401 (15)	0.4429 (2)	0.0152 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0114 (2)	0.0123 (2)	0.0181 (2)	−0.00059 (15)	0.00195 (17)	0.00469 (16)
Cu2	0.01222 (16)	0.01216 (15)	0.01634 (17)	0.00004 (10)	0.00307 (12)	0.00049 (11)
Cl1	0.0282 (3)	0.0268 (3)	0.0169 (3)	0.0022 (3)	0.0081 (3)	0.0001 (3)
O1	0.0138 (8)	0.0133 (8)	0.0197 (9)	−0.0007 (6)	−0.0016 (7)	0.0035 (7)
O2	0.0151 (9)	0.0141 (8)	0.0297 (10)	−0.0003 (6)	0.0110 (8)	0.0025 (7)
N1	0.0147 (10)	0.0151 (10)	0.0164 (11)	−0.0005 (8)	0.0049 (9)	0.0001 (8)
N2	0.0157 (10)	0.0145 (10)	0.0157 (11)	−0.0019 (8)	0.0022 (9)	−0.0001 (9)
C1	0.0096 (11)	0.0198 (12)	0.0169 (13)	−0.0009 (9)	0.0047 (10)	0.0066 (10)
C2	0.0146 (12)	0.0189 (12)	0.0228 (13)	−0.0008 (9)	0.0067 (10)	0.0034 (11)
C3	0.0182 (12)	0.0244 (13)	0.0213 (14)	−0.0060 (10)	0.0053 (11)	−0.0019 (11)
C4	0.0167 (12)	0.0304 (15)	0.0182 (14)	−0.0028 (10)	0.0030 (11)	0.0053 (11)
C5	0.0132 (12)	0.0218 (13)	0.0246 (14)	0.0018 (9)	0.0057 (11)	0.0070 (11)

C6	0.0104 (11)	0.0176 (12)	0.0213 (13)	−0.0012 (9)	0.0072 (10)	0.0029 (10)
C7	0.0129 (11)	0.0194 (12)	0.0254 (14)	0.0031 (9)	0.0075 (11)	0.0021 (11)
C8	0.0238 (13)	0.0155 (12)	0.0207 (14)	0.0045 (10)	0.0053 (11)	−0.0033 (10)
C9	0.0266 (14)	0.0148 (12)	0.0228 (14)	0.0011 (10)	0.0061 (12)	−0.0037 (10)
C10	0.0210 (13)	0.0153 (12)	0.0233 (14)	−0.0041 (10)	0.0020 (11)	−0.0055 (11)
C11	0.0133 (12)	0.0212 (12)	0.0209 (14)	−0.0010 (9)	0.0019 (10)	0.0012 (10)
C12	0.0138 (11)	0.0181 (12)	0.0140 (12)	0.0012 (9)	0.0010 (10)	0.0034 (10)
C13	0.0136 (12)	0.0247 (14)	0.0198 (13)	−0.0014 (10)	0.0028 (10)	0.0046 (11)
C14	0.0167 (12)	0.0313 (14)	0.0222 (14)	0.0048 (11)	0.0094 (11)	0.0085 (12)
C15	0.0239 (13)	0.0205 (13)	0.0177 (13)	0.0079 (10)	0.0067 (11)	0.0023 (10)
C16	0.0170 (12)	0.0169 (12)	0.0178 (13)	0.0004 (9)	0.0026 (10)	0.0036 (10)
C17	0.0125 (11)	0.0185 (12)	0.0139 (12)	0.0023 (9)	0.0027 (10)	0.0060 (10)

Geometric parameters (Å, º)

Cu2—Cl1	2.5092 (7)	C7—H7B	0.9900
Cu2—Cu1	2.9138 (3)	C8—N1	1.483 (3)
Cu1—O2^{i}	1.9108 (16)	C8—C9	1.520 (4)
Cu1—O1^{i}	1.9191 (15)	C8—H8A	0.9900
Cu1—Cu2^{i}	2.9138 (3)	C8—H8B	0.9900
O1—Cu1	1.9191 (15)	C9—C10	1.517 (3)
O1—Cu2	1.9825 (16)	C9—H9A	0.9900
O2—Cu1	1.9108 (16)	C9—H9B	0.9900
O2—Cu2	1.9632 (16)	C10—N2	1.488 (3)
N1—Cu2	1.995 (2)	C10—H10A	0.9900
N1—H1A	0.82 (3)	C10—H10B	0.9900
N2—Cu2	1.995 (2)	C11—N2	1.490 (3)
N2—H2A	0.86 (3)	C11—C12	1.505 (3)
C1—O1	1.351 (3)	C11—H11A	0.9900
C1—C2	1.392 (3)	C11—H11B	0.9900
C1—C6	1.408 (3)	C12—C13	1.394 (3)
C2—C3	1.386 (3)	C12—C17	1.406 (3)
C2—H2	0.9500	C13—C14	1.376 (4)
C3—C4	1.386 (4)	C13—H13	0.9500
C3—H3	0.9500	C14—C15	1.373 (4)
C4—C5	1.390 (4)	C14—H14	0.9500
C4—H4	0.9500	C15—C16	1.389 (3)
C5—C6	1.389 (3)	C15—H15	0.9500
C5—H5	0.9500	C16—C17	1.393 (3)
C6—C7	1.493 (3)	C16—H16	0.9500
C7—N1	1.489 (3)	C17—O2	1.353 (3)
C7—H7A	0.9900		

O2—Cu1—O2^{i}	180.00 (10)	C3—C4—C5	119.2 (2)
O2—Cu1—O1	80.93 (7)	C3—C4—H4	120.4
O2^{i}—Cu1—O1	99.07 (7)	C5—C4—H4	120.4
O2—Cu1—O1^{i}	99.07 (7)	C6—C5—C4	121.3 (2)
O2^{i}—Cu1—O1^{i}	80.93 (7)	C6—C5—H5	119.4

O1—Cu1—O1^{i}	180.0	C4—C5—H5	119.4
O2—Cu1—Cu2	41.91 (5)	C5—C6—C1	118.5 (2)
O2^{i}—Cu1—Cu2	138.09 (5)	C5—C6—C7	122.3 (2)
O1—Cu1—Cu2	42.52 (5)	C1—C6—C7	119.1 (2)
O1^{i}—Cu1—Cu2	137.48 (5)	N1—C7—C6	113.15 (19)
O2—Cu1—Cu2^{i}	138.09 (5)	N1—C7—H7A	108.9
O2^{i}—Cu1—Cu2^{i}	41.91 (5)	C6—C7—H7A	108.9
O1—Cu1—Cu2^{i}	137.48 (5)	N1—C7—H7B	109.0
O1^{i}—Cu1—Cu2^{i}	42.52 (5)	C6—C7—H7B	108.9
Cu2—Cu1—Cu2^{i}	180.000 (11)	H7A—C7—H7B	107.8
O2—Cu2—O1	78.09 (7)	N1—C8—C9	112.4 (2)
O2—Cu2—N1	163.99 (8)	N1—C8—H8A	109.1
O1—Cu2—N1	92.91 (7)	C9—C8—H8A	109.1
O2—Cu2—N2	93.17 (7)	N1—C8—H8B	109.1
O1—Cu2—N2	168.74 (8)	C9—C8—H8B	109.1
N1—Cu2—N2	93.87 (8)	H8A—C8—H8B	107.9
O2—Cu2—Cl1	89.92 (5)	C10—C9—C8	116.0 (2)
O1—Cu2—Cl1	88.09 (5)	C10—C9—H9A	108.3
N1—Cu2—Cl1	103.12 (6)	C8—C9—H9A	108.3
N2—Cu2—Cl1	99.10 (6)	C10—C9—H9B	108.3
O2—Cu2—Cu1	40.55 (5)	C8—C9—H9B	108.3
O1—Cu2—Cu1	40.86 (4)	H9A—C9—H9B	107.4
N1—Cu2—Cu1	133.49 (6)	N2—C10—C9	113.1 (2)
N2—Cu2—Cu1	132.54 (6)	N2—C10—H10A	109.0
Cl1—Cu2—Cu1	76.178 (16)	C9—C10—H10A	109.0
C1—O1—Cu1	129.48 (14)	N2—C10—H10B	109.0
C1—O1—Cu2	120.13 (13)	C9—C10—H10B	109.0
Cu1—O1—Cu2	96.62 (7)	H10A—C10—H10B	107.8
C17—O2—Cu1	133.74 (15)	N2—C11—C12	114.1 (2)
C17—O2—Cu2	125.53 (14)	N2—C11—H11A	108.7
Cu1—O2—Cu2	97.54 (7)	C12—C11—H11A	108.7
C8—N1—C7	111.16 (19)	N2—C11—H11B	108.7
C8—N1—Cu2	112.34 (15)	C12—C11—H11B	108.7
C7—N1—Cu2	112.63 (15)	H11A—C11—H11B	107.6
C8—N1—H1A	107 (2)	C13—C12—C17	118.5 (2)
C7—N1—H1A	110 (2)	C13—C12—C11	122.5 (2)
Cu2—N1—H1A	103 (2)	C17—C12—C11	118.8 (2)
C10—N2—C11	109.87 (19)	C14—C13—C12	121.1 (2)
C10—N2—Cu2	112.19 (15)	C14—C13—H13	119.4
C11—N2—Cu2	111.40 (15)	C12—C13—H13	119.4
C10—N2—H2A	106.1 (19)	C15—C14—C13	119.9 (2)
C11—N2—H2A	109.0 (19)	C15—C14—H14	120.1
Cu2—N2—H2A	108 (2)	C13—C14—H14	120.1
O1—C1—C2	122.5 (2)	C14—C15—C16	120.9 (2)
O1—C1—C6	117.0 (2)	C14—C15—H15	119.5
C2—C1—C6	120.5 (2)	C16—C15—H15	119.5
C3—C2—C1	119.5 (2)	C15—C16—C17	119.3 (2)
C3—C2—H2	120.3	C15—C16—H16	120.3

C1—C2—H2	120.3	C17—C16—H16	120.3
C2—C3—C4	121.0 (2)	O2—C17—C16	122.2 (2)
C2—C3—H3	119.5	O2—C17—C12	117.6 (2)
C4—C3—H3	119.5	C16—C17—C12	120.2 (2)
O1—C1—C2—C3	−178.7 (2)	C1—O1—Cu2—N2	−84.8 (4)
C6—C1—C2—C3	1.3 (3)	Cu1—O1—Cu2—N2	59.1 (4)
C1—C2—C3—C4	0.1 (4)	C1—O1—Cu2—Cl1	145.23 (16)
C2—C3—C4—C5	−0.5 (4)	Cu1—O1—Cu2—Cl1	−70.93 (6)
C3—C4—C5—C6	−0.4 (4)	C1—O1—Cu2—Cu1	−143.8 (2)
C4—C5—C6—C1	1.7 (4)	C8—N1—Cu2—O2	−168.1 (2)
C4—C5—C6—C7	−175.4 (2)	C7—N1—Cu2—O2	65.5 (3)
O1—C1—C6—C5	177.8 (2)	C8—N1—Cu2—O1	136.78 (16)
C2—C1—C6—C5	−2.1 (3)	C7—N1—Cu2—O1	10.33 (17)
O1—C1—C6—C7	−5.0 (3)	C8—N1—Cu2—N2	−52.22 (17)
C2—C1—C6—C7	175.0 (2)	C7—N1—Cu2—N2	−178.67 (17)
C5—C6—C7—N1	−119.7 (2)	C8—N1—Cu2—Cl1	48.06 (16)
C1—C6—C7—N1	63.2 (3)	C7—N1—Cu2—Cl1	−78.39 (16)
N1—C8—C9—C10	−64.3 (3)	C8—N1—Cu2—Cu1	131.34 (14)
C8—C9—C10—N2	63.9 (3)	C7—N1—Cu2—Cu1	4.9 (2)
N2—C11—C12—C13	122.6 (2)	C10—N2—Cu2—O2	−143.06 (16)
N2—C11—C12—C17	−61.6 (3)	C11—N2—Cu2—O2	−19.41 (17)
C17—C12—C13—C14	−1.6 (4)	C10—N2—Cu2—O1	178.2 (3)
C11—C12—C13—C14	174.2 (2)	C11—N2—Cu2—O1	−58.1 (5)
C12—C13—C14—C15	0.5 (4)	C10—N2—Cu2—N1	51.32 (17)
C13—C14—C15—C16	0.7 (4)	C11—N2—Cu2—N1	174.98 (17)
C14—C15—C16—C17	−0.7 (4)	C10—N2—Cu2—Cl1	−52.64 (16)
C15—C16—C17—O2	179.0 (2)	C11—N2—Cu2—Cl1	71.02 (16)
C15—C16—C17—C12	−0.4 (3)	C10—N2—Cu2—Cu1	−132.18 (14)
C13—C12—C17—O2	−177.9 (2)	C11—N2—Cu2—Cu1	−8.5 (2)
C11—C12—C17—O2	6.1 (3)	C17—O2—Cu1—O1	−139.7 (2)
C13—C12—C17—C16	1.5 (3)	Cu2—O2—Cu1—O1	20.00 (8)
C11—C12—C17—C16	−174.5 (2)	C17—O2—Cu1—O1^{i}	40.3 (2)
C9—C8—N1—C7	−170.9 (2)	Cu2—O2—Cu1—O1^{i}	−160.00 (8)
C9—C8—N1—Cu2	61.9 (2)	C17—O2—Cu1—Cu2	−159.7 (3)
C6—C7—N1—C8	176.1 (2)	C17—O2—Cu1—Cu2^{i}	20.3 (3)
C6—C7—N1—Cu2	−56.8 (2)	Cu2—O2—Cu1—Cu2^{i}	180.0
C9—C10—N2—C11	174.7 (2)	C1—O1—Cu1—O2	118.85 (19)
C9—C10—N2—Cu2	−60.8 (2)	Cu2—O1—Cu1—O2	−19.76 (8)
C12—C11—N2—C10	−173.3 (2)	C1—O1—Cu1—O2^{i}	−61.15 (19)
C12—C11—N2—Cu2	61.7 (2)	Cu2—O1—Cu1—O2^{i}	160.24 (8)
C2—C1—O1—Cu1	0.6 (3)	C1—O1—Cu1—Cu2	138.6 (2)
C6—C1—O1—Cu1	−179.40 (15)	C1—O1—Cu1—Cu2^{i}	−41.4 (2)
C2—C1—O1—Cu2	131.2 (2)	Cu2—O1—Cu1—Cu2^{i}	180.0
C6—C1—O1—Cu2	−48.8 (3)	O1—Cu2—Cu1—O2	150.01 (11)
C16—C17—O2—Cu1	15.6 (3)	N1—Cu2—Cu1—O2	158.32 (12)
C12—C17—O2—Cu1	−164.97 (17)	N2—Cu2—Cu1—O2	−16.86 (11)
C16—C17—O2—Cu2	−139.41 (19)	Cl1—Cu2—Cu1—O2	−106.58 (8)

C12—C17—O2—Cu2	40.0 (3)	O2—Cu2—Cu1—O2^{i}	180.0
C17—O2—Cu2—O1	142.55 (19)	O1—Cu2—Cu1—O2^{i}	−29.99 (11)
Cu1—O2—Cu2—O1	−19.52 (7)	N1—Cu2—Cu1—O2^{i}	−21.68 (12)
C17—O2—Cu2—N1	85.7 (3)	N2—Cu2—Cu1—O2^{i}	163.14 (11)
Cu1—O2—Cu2—N1	−76.4 (3)	Cl1—Cu2—Cu1—O2^{i}	73.42 (8)
C17—O2—Cu2—N2	−30.28 (19)	O2—Cu2—Cu1—O1	−150.01 (11)
Cu1—O2—Cu2—N2	167.64 (8)	N1—Cu2—Cu1—O1	8.31 (11)
C17—O2—Cu2—Cl1	−129.39 (18)	N2—Cu2—Cu1—O1	−166.86 (11)
Cu1—O2—Cu2—Cl1	68.54 (6)	Cl1—Cu2—Cu1—O1	103.41 (8)
C17—O2—Cu2—Cu1	162.1 (2)	O2—Cu2—Cu1—O1^{i}	29.99 (11)
C1—O1—Cu2—O2	−124.44 (17)	O1—Cu2—Cu1—O1^{i}	180.0
Cu1—O1—Cu2—O2	19.40 (7)	N1—Cu2—Cu1—O1^{i}	−171.69 (11)
C1—O1—Cu2—N1	42.19 (17)	N2—Cu2—Cu1—O1^{i}	13.14 (11)
Cu1—O1—Cu2—N1	−173.97 (8)	Cl1—Cu2—Cu1—O1^{i}	−76.59 (8)

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