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[2,2′-Dihydroxy-N^2,$N^{2'}$-(3-hydroxyimino-pentane-2,4-diyl)dibenzohydrazidato]-copper(II)

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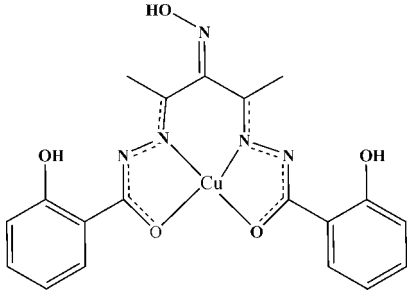
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; H-atom completeness 95%; disorder in main residue; R factor = 0.034; wR factor = 0.079; data-to-parameter ratio = 15.7.

The Cu^{II} atom in the title complex, $[Cu(C_{19}H_{17}N_5O_5)]$, is coordinated by two N atoms and two O atoms of one 2,2′-dihydroxy-N^2,$N^{2'}$-(3-hydroxyiminopentane-2,4-diyl)dibenzohydrazidate ligand, exhibiting a distorted square-planar geometry. The dihedral angle between the two benzene rings in the oxime hydrazone is 7.62 (15)°. The molecular configuration is stabilized by intramolecular O—H···N hydrogen bonds. Pairs of centrosymmetrically related molecules are linked into dimers by two intermolecular C—H···O hydrogen bonds. Each dimer is further connected to four neighboring dimers *via* four O—H···O hydrogen bonds, forming an extended two-dimensional structure. The oxime O atom is disordered over two orientations in a 2:1 ratio.

Related literature

For the structural versatility and biological activity of oxime hydrazone compounds and their metal complexes, see: Marmion *et al.* (2004); Song *et al.* (2000); Xiao *et al.* (2004). For similar copper(II) complexes with Schiff bases, see: Suleiman Gwaram *et al.* (2010); Qin *et al.* (2010).



Experimental

Crystal data

$[Cu(C_{19}H_{17}N_5O_5)]$
M_r = 458.92
Monoclinic, $P2_1/n$
a = 8.7672 (5) Å
b = 19.0262 (11) Å
c = 11.6118 (6) Å
β = 91.437 (2)°
V = 1936.31 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 293 K
0.52 × 0.22 × 0.15 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.715, T_{max} = 0.833
17167 measured reflections
4436 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 0.91
4436 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	1.86	2.586 (2)	147
O5—H5B···N5	0.82	1.79	2.519 (2)	148
C19—H19A···O2^{i}	0.96	2.58	3.525 (3)	170
O3A···O5^{ii}			2.643 (3)	

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEX* (McArdle, 1995); 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: OM2355).

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supporting information

Acta Cryst. (2010). E**66**, m1422 [https://doi.org/10.1107/S1600536810040754]

[2,2′-Dihydroxy-N^2,$N^{2'}$-(3-hydroxyiminopentane-2,4-diyl)dibenzohydrazidato]copper(II)

Zi-Jing Xiao

S1. Comment

Recently, much attention has been focused on oxime compounds and their complexes, due to their biological activities, chemical and industrial versatility, and excellent chelating capability (Marmion, *et al.*, 2004; Song *et al.*, 2000; Xiao, *et al.*, 2004). Oxime hydrazone and hydroxamic acids are the two kinds of oxime compounds. Herein, we present the synthesis and structure of copper complex with 2,2′-dihydroxy-N^2,$N^{2'}$-(3-hydroxyiminopentane- 2,4-diyl)dibenzohydrazide.

As shown in Figure 1, the copper atom in the title complex has a square-planar coordination geometry, the four donors are two hydrazine nitrogen atoms and two carboxyl oxygen atoms in the oxime hydrazone ligand. The bond lengths of Cu-N and Cu-O in the square planar complex are similar to those in this type of copper complex (Suleiman Gwaram *et al.*, 2010; Qin *et al.*, 2010). The whole oxime hydrazone ligand is not planar; the dihedral angle between the two benzene rings in the oxime hydrazone ligand is 7.62 (15)°.

There are intramolecular O-H ···N hydrogen bonds, and intermolecular oxime-phenol O-H···O hydrogen bonds and intermolecular C-H···O hydrogen bonds in the title complex. The interatomic distance of O3A – $O5^{ii}$ (symmetry code ii, 1/2+x, 1/2-y, 1/2+z) is 2.643 (3)Å. It means that there may exist O-H (oxime group) ···O (phenol) hydrogen bonds, although the hydrogen atom in N-O-H has not been found. These intermolecular O-H···O and C-H···O hydrogen bonds result in an extended two-dimensional layer structure (see Figure 2).

S2. Experimental

Solid $CuBr_2$ (0.0477g, 0.2 mmol) was dissolved in 12 mL of methanol to get solution A. 2, 3, 4-pentanetrione-3-oxime (0.0258g, 0.2 mmol) and salicyloyl hydrazine (0.0304g, 0.2 mmol) were dissolved in 12 mL of methanol to get solution B. To the solution B was added the solution A slowly. The reaction mixture was stirred and refluxed for 2 hours to give a green solution. The deep blue crystals of the title complex were formed upon slow evaporation at about 297 K after 20 d.

S3. Refinement

On the residial density there is one peak, 2.24 e Å3, corresponding to a second position for the O3 atom. The treatment of the disorder shows that the O3 atom in the N3-O3 oxime group is disordered over two postions as O3A and O3B in ratio 2/1. The oxime group-bound H atom was not found in the difference Fourier map. All other H atoms were placed in calculated positions and refined using a riding model [C-H = 0.93 Å and Uiso(H) = 1.2Ueq(C) for aromatic H atoms, C-H = 0.96 Å and Uiso(H) = 1.5Ueq(C) for methyl H atoms, and O-H = 0.82 Å and Uiso(H) = 1.2Ueq(O)].

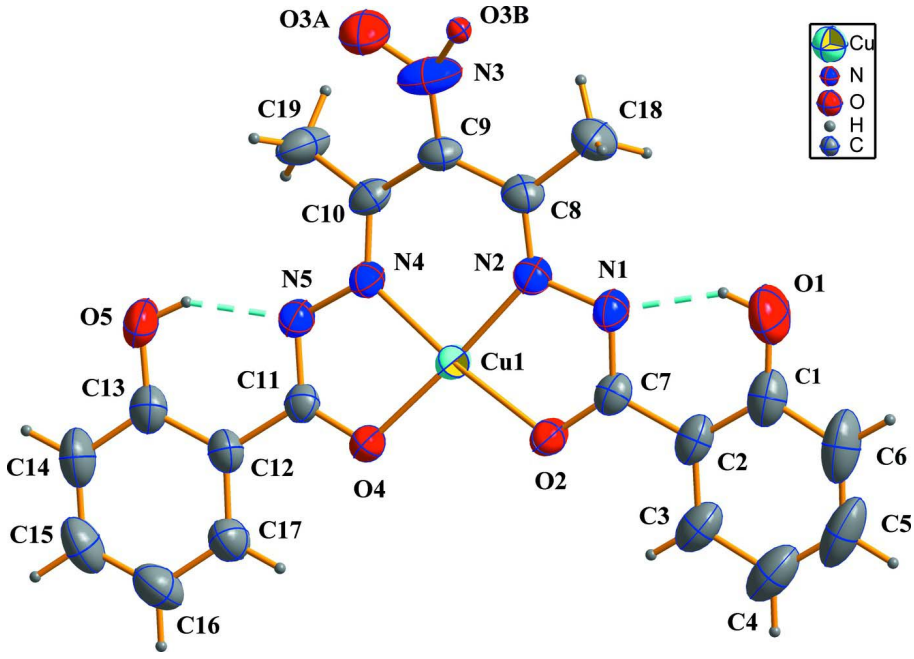

Figure 1

The molecular structure of the title complex, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate intramolecular hydrogen bonding.

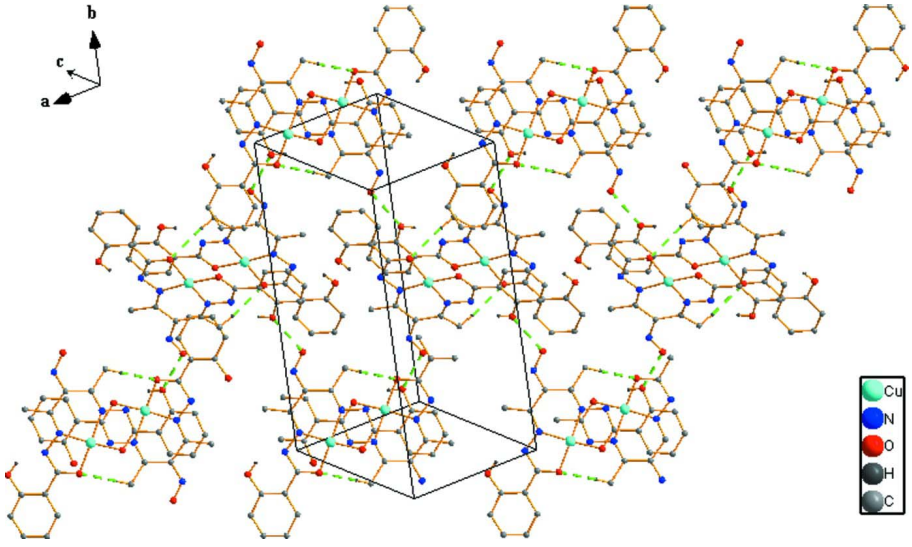

Figure 2

The extended two-dimensional layer of the title complex, dotted green lines represent intermolecular hydrogen bonding. Only H atoms participating in hydrogen bonds are shown.

[2,2′-Dihydroxy-*N*^{2},*N*$^{2'}$-(3-hydroxyiminopentane- 2,4-diyl)dibenzohydrazidato]copper(II)

Crystal data

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Hall symbol: -P 2yn
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c = 11.6118 (6) Å
β = 91.437 (2)°
V = 1936.31 (19) Å^3
Z = 4
F(000) = 940
D_x = 1.574 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 4577 reflections
θ = 2.1–27.5°
μ = 1.17 mm^{-1}
T = 293 K
Prism, blue
0.52 × 0.22 × 0.15 mm

Data collection

Rigaku Weissenberg IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.715, T_{max} = 0.833

17167 measured reflections
4436 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.5°, θ_{min} = 2.1°
h = 0→11
k = −24→24
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 0.91
4436 reflections
282 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}	Occ. (<1)
Cu1	0.24832 (3)	0.508624 (12)	0.47601 (2)	0.03770 (9)	
N1	0.46486 (19)	0.53298 (9)	0.64875 (15)	0.0428 (4)	
N2	0.36561 (18)	0.48024 (9)	0.61023 (14)	0.0380 (4)	
N3	0.2905 (3)	0.30306 (12)	0.6725 (2)	0.0735 (7)	
N4	0.13118 (18)	0.42316 (8)	0.47217 (14)	0.0364 (4)	
N5	0.01862 (18)	0.42494 (9)	0.38607 (15)	0.0401 (4)	
O1	0.6627 (2)	0.59621 (11)	0.78120 (17)	0.0805 (6)	
H1A	0.6074	0.5640	0.7587	0.097*	
O2	0.34881 (15)	0.59685 (7)	0.50147 (13)	0.0414 (3)	

O3A	0.2209 (4)	0.24814 (15)	0.6492 (3)	0.0749 (8)	0.67
O3B	0.3899 (6)	0.2757 (2)	0.7190 (5)	0.0635 (15)	0.33
O4	0.12933 (16)	0.53067 (7)	0.33856 (12)	0.0414 (3)	
O5	−0.16592 (19)	0.36688 (8)	0.24617 (14)	0.0604 (5)	
H5B	−0.1070	0.3703	0.3019	0.072*	
C1	0.6346 (3)	0.65344 (14)	0.7173 (2)	0.0581 (7)	
C2	0.5294 (2)	0.65449 (12)	0.6241 (2)	0.0461 (5)	
C3	0.5081 (3)	0.71686 (12)	0.5633 (2)	0.0594 (7)	
H3A	0.4376	0.7182	0.5022	0.071*	
C4	0.5894 (3)	0.77687 (15)	0.5916 (3)	0.0784 (9)	
H4A	0.5743	0.8181	0.5498	0.094*	
C5	0.6921 (4)	0.77491 (18)	0.6816 (3)	0.0911 (11)	
H5A	0.7467	0.8153	0.7011	0.109*	
C6	0.7166 (3)	0.71460 (19)	0.7439 (3)	0.0849 (10)	
H6A	0.7882	0.7144	0.8044	0.102*	
C7	0.4416 (2)	0.59175 (11)	0.58840 (18)	0.0386 (5)	
C8	0.3669 (2)	0.42120 (11)	0.66539 (18)	0.0409 (5)	
C9	0.2605 (2)	0.36376 (11)	0.62829 (19)	0.0405 (5)	
C10	0.1317 (2)	0.37065 (10)	0.54304 (19)	0.0394 (5)	
C11	0.0336 (2)	0.48128 (10)	0.31893 (17)	0.0355 (4)	
C12	−0.0688 (2)	0.48412 (11)	0.21619 (17)	0.0402 (5)	
C13	−0.1615 (3)	0.42678 (13)	0.1830 (2)	0.0485 (5)	
C14	−0.2529 (3)	0.43151 (16)	0.0835 (2)	0.0647 (7)	
H14A	−0.3146	0.3939	0.0613	0.078*	
C15	−0.2519 (3)	0.49149 (17)	0.0182 (2)	0.0718 (8)	
H15A	−0.3126	0.4939	−0.0485	0.086*	
C16	−0.1628 (3)	0.54807 (16)	0.0496 (2)	0.0679 (7)	
H16A	−0.1637	0.5886	0.0047	0.082*	
C17	−0.0720 (3)	0.54442 (13)	0.14814 (19)	0.0510 (6)	
H17A	−0.0120	0.5828	0.1695	0.061*	
C18	0.4736 (3)	0.41084 (14)	0.7671 (2)	0.0635 (7)	
H18A	0.4647	0.4498	0.8190	0.095*	
H18B	0.5765	0.4079	0.7412	0.095*	
H18C	0.4478	0.3682	0.8062	0.095*	
C19	0.0055 (3)	0.31770 (13)	0.5377 (3)	0.0628 (7)	
H19A	−0.0886	0.3407	0.5167	0.094*	
H19B	−0.0038	0.2958	0.6117	0.094*	
H19C	0.0278	0.2826	0.4812	0.094*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03850 (14)	0.03025 (14)	0.04393 (15)	−0.00304 (11)	−0.00734 (9)	0.00278 (11)
N1	0.0401 (9)	0.0385 (10)	0.0495 (11)	−0.0008 (8)	−0.0091 (8)	−0.0045 (8)
N2	0.0340 (8)	0.0354 (10)	0.0443 (10)	0.0032 (7)	−0.0031 (7)	−0.0007 (8)
N3	0.0906 (18)	0.0425 (13)	0.0885 (18)	0.0125 (12)	0.0220 (14)	0.0210 (12)
N4	0.0365 (9)	0.0305 (9)	0.0418 (10)	0.0005 (7)	−0.0045 (7)	−0.0002 (7)
N5	0.0402 (9)	0.0339 (9)	0.0459 (10)	−0.0028 (7)	−0.0059 (8)	−0.0011 (8)

O1	0.0776 (13)	0.0845 (15)	0.0776 (14)	−0.0080 (11)	−0.0329 (11)	−0.0108 (11)
O2	0.0395 (8)	0.0317 (8)	0.0527 (9)	−0.0020 (6)	−0.0074 (7)	0.0017 (6)
O3A	0.093 (2)	0.0467 (17)	0.084 (2)	0.0043 (15)	−0.0252 (17)	0.0092 (14)
O3B	0.072 (3)	0.037 (3)	0.079 (4)	0.012 (2)	−0.045 (3)	0.014 (2)
O4	0.0468 (8)	0.0340 (8)	0.0430 (8)	−0.0071 (7)	−0.0071 (6)	0.0029 (6)
O5	0.0683 (11)	0.0463 (10)	0.0655 (11)	−0.0133 (8)	−0.0179 (9)	−0.0114 (8)
C1	0.0483 (14)	0.0602 (17)	0.0656 (17)	−0.0051 (12)	−0.0011 (12)	−0.0208 (13)
C2	0.0377 (11)	0.0423 (13)	0.0586 (14)	−0.0036 (10)	0.0049 (10)	−0.0157 (11)
C3	0.0614 (16)	0.0400 (14)	0.0772 (18)	−0.0083 (12)	0.0089 (13)	−0.0106 (12)
C4	0.083 (2)	0.0457 (16)	0.107 (3)	−0.0180 (15)	0.0168 (19)	−0.0154 (16)
C5	0.083 (2)	0.068 (2)	0.123 (3)	−0.0347 (18)	0.013 (2)	−0.040 (2)
C6	0.0618 (19)	0.094 (3)	0.098 (2)	−0.0187 (18)	−0.0068 (17)	−0.044 (2)
C7	0.0328 (10)	0.0360 (11)	0.0471 (13)	0.0016 (8)	0.0023 (9)	−0.0067 (9)
C8	0.0383 (11)	0.0382 (11)	0.0461 (13)	0.0094 (9)	−0.0020 (9)	0.0026 (9)
C9	0.0414 (11)	0.0332 (11)	0.0468 (12)	0.0057 (9)	0.0012 (9)	0.0072 (9)
C10	0.0377 (11)	0.0288 (10)	0.0517 (13)	0.0036 (8)	0.0040 (9)	0.0010 (9)
C11	0.0362 (10)	0.0325 (10)	0.0377 (11)	0.0030 (8)	−0.0009 (8)	−0.0051 (8)
C12	0.0394 (11)	0.0439 (12)	0.0370 (11)	0.0012 (9)	−0.0011 (8)	−0.0068 (9)
C13	0.0475 (13)	0.0499 (14)	0.0479 (13)	−0.0009 (10)	−0.0040 (10)	−0.0118 (11)
C14	0.0592 (15)	0.076 (2)	0.0583 (16)	−0.0082 (14)	−0.0143 (12)	−0.0202 (15)
C15	0.0670 (17)	0.098 (2)	0.0495 (14)	−0.0008 (17)	−0.0213 (12)	−0.0039 (16)
C16	0.0711 (17)	0.082 (2)	0.0497 (15)	0.0027 (16)	−0.0104 (13)	0.0140 (14)
C17	0.0506 (13)	0.0555 (15)	0.0466 (13)	−0.0031 (11)	−0.0061 (10)	0.0035 (11)
C18	0.0716 (17)	0.0571 (16)	0.0605 (16)	0.0002 (13)	−0.0220 (13)	0.0119 (13)
C19	0.0526 (14)	0.0424 (14)	0.093 (2)	−0.0080 (11)	−0.0113 (14)	0.0233 (13)

Geometric parameters (Å, º)

Cu1—O2	1.9153 (13)	C4—C5	1.362 (4)
Cu1—N2	1.9230 (16)	C4—H4A	0.9300
Cu1—N4	1.9231 (16)	C5—C6	1.371 (5)
Cu1—O4	1.9308 (14)	C5—H5A	0.9300
N1—C7	1.333 (3)	C6—H6A	0.9300
N1—N2	1.395 (2)	C8—C9	1.493 (3)
N2—C8	1.293 (3)	C8—C18	1.501 (3)
N3—O3B	1.140 (4)	C9—C10	1.489 (3)
N3—O3A	1.236 (3)	C10—C19	1.497 (3)
N3—C9	1.288 (3)	C11—C12	1.476 (3)
N4—C10	1.294 (3)	C12—C17	1.393 (3)
N4—N5	1.388 (2)	C12—C13	1.408 (3)
N5—C11	1.334 (3)	C13—C14	1.392 (3)
O1—C1	1.337 (3)	C14—C15	1.370 (4)
O1—H1A	0.8200	C14—H14A	0.9300
O2—C7	1.284 (2)	C15—C16	1.374 (4)
O3A—O3B	1.752 (5)	C15—H15A	0.9300
O4—C11	1.277 (2)	C16—C17	1.379 (3)
O5—C13	1.356 (3)	C16—H16A	0.9300
O5—H5B	0.8200	C17—H17A	0.9300

C1—C6	1.398 (4)	C18—H18A	0.9600
C1—C2	1.404 (3)	C18—H18B	0.9600
C2—C3	1.391 (3)	C18—H18C	0.9600
C2—C7	1.474 (3)	C19—H19A	0.9600
C3—C4	1.381 (3)	C19—H19B	0.9600
C3—H3A	0.9300	C19—H19C	0.9600

O2—Cu1—N2	83.48 (6)	N2—C8—C9	119.70 (18)
O2—Cu1—N4	171.09 (7)	N2—C8—C18	120.1 (2)
N2—Cu1—N4	93.19 (7)	C9—C8—C18	120.22 (19)
O2—Cu1—O4	100.02 (6)	N3—C9—C10	119.2 (2)
N2—Cu1—O4	176.23 (6)	N3—C9—C8	114.9 (2)
N4—Cu1—O4	83.54 (6)	C10—C9—C8	125.81 (18)
C7—N1—N2	110.44 (16)	N4—C10—C9	118.78 (18)
C8—N2—N1	117.96 (17)	N4—C10—C19	120.15 (19)
C8—N2—Cu1	130.03 (15)	C9—C10—C19	121.07 (19)
N1—N2—Cu1	111.99 (13)	O4—C11—N5	124.12 (18)
O3B—N3—O3A	94.9 (3)	O4—C11—C12	120.09 (18)
O3B—N3—C9	138.1 (4)	N5—C11—C12	115.79 (18)
O3A—N3—C9	125.1 (3)	C17—C12—C13	118.7 (2)
C10—N4—N5	117.91 (17)	C17—C12—C11	119.46 (19)
C10—N4—Cu1	130.13 (14)	C13—C12—C11	121.9 (2)
N5—N4—Cu1	111.46 (12)	O5—C13—C14	118.6 (2)
C11—N5—N4	111.23 (16)	O5—C13—C12	121.8 (2)
C1—O1—H1A	109.5	C14—C13—C12	119.5 (2)
C7—O2—Cu1	109.58 (13)	C15—C14—C13	120.1 (2)
C11—O4—Cu1	109.08 (13)	C15—C14—H14A	119.9
C13—O5—H5B	109.5	C13—C14—H14A	119.9
O1—C1—C6	117.9 (3)	C14—C15—C16	121.1 (2)
O1—C1—C2	123.2 (2)	C14—C15—H15A	119.4
C6—C1—C2	118.9 (3)	C16—C15—H15A	119.4
C3—C2—C1	118.7 (2)	C15—C16—C17	119.6 (3)
C3—C2—C7	119.0 (2)	C15—C16—H16A	120.2
C1—C2—C7	122.2 (2)	C17—C16—H16A	120.2
C4—C3—C2	121.5 (3)	C16—C17—C12	121.0 (2)
C4—C3—H3A	119.2	C16—C17—H17A	119.5
C2—C3—H3A	119.2	C12—C17—H17A	119.5
C5—C4—C3	119.1 (3)	C8—C18—H18A	109.5
C5—C4—H4A	120.4	C8—C18—H18B	109.5
C3—C4—H4A	120.4	H18A—C18—H18B	109.5
C4—C5—C6	121.3 (3)	C8—C18—H18C	109.5
C4—C5—H5A	119.3	H18A—C18—H18C	109.5
C6—C5—H5A	119.3	H18B—C18—H18C	109.5
C5—C6—C1	120.5 (3)	C10—C19—H19A	109.5
C5—C6—H6A	119.8	C10—C19—H19B	109.5
C1—C6—H6A	119.8	H19A—C19—H19B	109.5
O2—C7—N1	124.22 (19)	C10—C19—H19C	109.5
O2—C7—C2	118.43 (19)	H19A—C19—H19C	109.5

N1—C7—C2	117.36 (19)	H19B—C19—H19C	109.5
C7—N1—N2—C8	−175.43 (18)	Cu1—N2—C8—C9	−2.6 (3)
C7—N1—N2—Cu1	5.9 (2)	N1—N2—C8—C18	−0.3 (3)
O2—Cu1—N2—C8	177.17 (19)	Cu1—N2—C8—C18	178.08 (16)
N4—Cu1—N2—C8	5.46 (19)	O3B—N3—C9—C10	160.8 (5)
O2—Cu1—N2—N1	−4.33 (12)	O3A—N3—C9—C10	0.8 (4)
N4—Cu1—N2—N1	−176.04 (13)	O3B—N3—C9—C8	−16.5 (6)
N2—Cu1—N4—C10	4.20 (19)	O3A—N3—C9—C8	−176.5 (3)
O4—Cu1—N4—C10	−177.69 (19)	N2—C8—C9—N3	166.7 (2)
N2—Cu1—N4—N5	175.78 (13)	C18—C8—C9—N3	−14.0 (3)
O4—Cu1—N4—N5	−6.10 (12)	N2—C8—C9—C10	−10.4 (3)
C10—N4—N5—C11	−179.12 (18)	C18—C8—C9—C10	168.9 (2)
Cu1—N4—N5—C11	8.1 (2)	N5—N4—C10—C9	173.72 (17)
N2—Cu1—O2—C7	1.81 (13)	Cu1—N4—C10—C9	−15.1 (3)
O4—Cu1—O2—C7	−176.79 (13)	N5—N4—C10—C19	−5.6 (3)
C9—N3—O3A—O3B	166.8 (5)	Cu1—N4—C10—C19	165.55 (17)
C9—N3—O3B—O3A	−163.7 (6)	N3—C9—C10—N4	−157.7 (2)
O2—Cu1—O4—C11	−169.01 (12)	C8—C9—C10—N4	19.3 (3)
N4—Cu1—O4—C11	2.74 (13)	N3—C9—C10—C19	21.6 (3)
O1—C1—C2—C3	179.8 (2)	C8—C9—C10—C19	−161.4 (2)
C6—C1—C2—C3	−1.4 (4)	Cu1—O4—C11—N5	1.5 (2)
O1—C1—C2—C7	−0.6 (4)	Cu1—O4—C11—C12	−178.11 (14)
C6—C1—C2—C7	178.3 (2)	N4—N5—C11—O4	−6.6 (3)
C1—C2—C3—C4	0.9 (4)	N4—N5—C11—C12	172.98 (16)
C7—C2—C3—C4	−178.7 (2)	O4—C11—C12—C17	−7.1 (3)
C2—C3—C4—C5	−0.4 (4)	N5—C11—C12—C17	173.30 (19)
C3—C4—C5—C6	0.3 (5)	O4—C11—C12—C13	171.42 (19)
C4—C5—C6—C1	−0.8 (5)	N5—C11—C12—C13	−8.2 (3)
O1—C1—C6—C5	−179.8 (3)	C17—C12—C13—O5	−178.9 (2)
C2—C1—C6—C5	1.3 (4)	C11—C12—C13—O5	2.6 (3)
Cu1—O2—C7—N1	1.3 (2)	C17—C12—C13—C14	0.3 (3)
Cu1—O2—C7—C2	−179.02 (15)	C11—C12—C13—C14	−178.2 (2)
N2—N1—C7—O2	−4.9 (3)	O5—C13—C14—C15	179.5 (2)
N2—N1—C7—C2	175.42 (17)	C12—C13—C14—C15	0.3 (4)
C3—C2—C7—O2	0.4 (3)	C13—C14—C15—C16	−0.6 (4)
C1—C2—C7—O2	−179.2 (2)	C14—C15—C16—C17	0.4 (4)
C3—C2—C7—N1	−179.9 (2)	C15—C16—C17—C12	0.2 (4)
C1—C2—C7—N1	0.4 (3)	C13—C12—C17—C16	−0.5 (3)
N1—N2—C8—C9	178.94 (17)	C11—C12—C17—C16	178.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1	0.82	1.86	2.586 (2)	147
O5—H5*B*···N5	0.82	1.79	2.519 (2)	148

C19—H19*A*···O2^{i}	0.96	2.58	3.525 (3)	170
O3*A*—H···O5^{ii}			2.643 (3)	

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+1/2, *z*+1/2.