

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(1*H*-Imidazole- κ N³){*N*-[1-(2-oxido-phenyl- κ O)ethylidene]-*L*-phenyl-alaninato- κ^2 N,O}copper(II)

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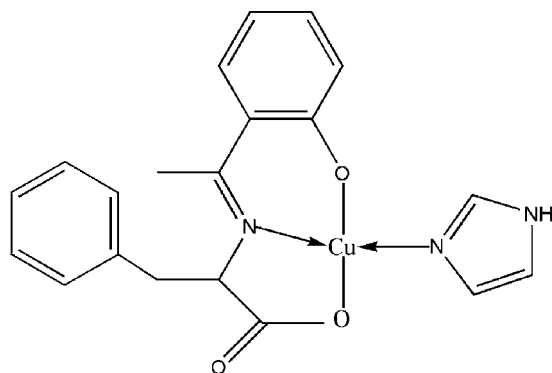
Received 19 August 2008; accepted 28 August 2008

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.029; wR factor = 0.067; data-to-parameter ratio = 14.4.

In the title compound, $[\text{Cu}(\text{C}_{17}\text{H}_{15}\text{NO}_3)(\text{C}_3\text{H}_4\text{N}_2)]$, the Cu^{II} atom is four-coordinated by two O atoms and the N atom of the tridentate Schiff base ligand, and one N atom from the imidazole ligand in a distorted square-planar geometry. In the crystal structure, molecules are linked into dimers by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related literature, see: Basu Baul *et al.* (2007); Casella & Guillotti (1983); Ganguly *et al.* (2008); Parekh *et al.* (2006); Plesch *et al.* (1997); Usman *et al.* (2003); Vigato & Tamburini (2004).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{17}\text{H}_{15}\text{NO}_3)(\text{C}_3\text{H}_4\text{N}_2)]$
 $M_r = 412.92$
 Orthorhombic, $C222_1$
 $a = 16.8029$ (16) Å
 $b = 19.8231$ (19) Å
 $c = 11.3642$ (11) Å

$V = 3785.3$ (6) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.18$ mm⁻¹
 $T = 291$ (2) K
 $0.43 \times 0.34 \times 0.25$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.630$, $T_{\text{max}} = 0.759$
 10101 measured reflections
 3534 independent reflections
 3008 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.067$
 $S = 1.01$
 3534 reflections
 245 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³
 Absolute structure: Flack (1983), 1557 Friedel pairs
 Flack parameter: -0.029 (12)

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.8876 (19)	Cu1—O3	1.9511 (18)
Cu1—N1	1.945 (2)	Cu1—N2	1.958 (2)
O1—Cu1—N1	93.33 (9)	O1—Cu1—N2	93.20 (9)
O1—Cu1—O3	171.74 (9)	N1—Cu1—N2	162.84 (10)
N1—Cu1—O3	84.90 (8)	O3—Cu1—N2	90.77 (8)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3D}\cdots\text{O2}^i$	0.86	1.95	2.789 (3)	166

Symmetry code: (i) $x, -y + 1, -z + 2$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This research was supported by the National Science Foundation of China (grant No. 20676057).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2661).

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supporting information

Acta Cryst. (2008). E64, m1228 [doi:10.1107/S160053680802758X]

(1*H*-Imidazole- κ N³){*N*-[1-(2-oxidophenyl- κ O)ethylidene]-*L*-phenylalaninato- κ^2 N,O}copper(II)

Yong-Jun Han, Gan-Qing Zhao, Xiao-Jun Zhao, Wen-Li Song and Jie-Li Shi

S1. Comment

In the past decades, significant progress has been achieved in understanding the chemistry of transition metal complexes with Schiff base ligands composed of salicylaldehyde, 2-formylpyridine or their analogues, and α -amino acids (Vigato & Tamburini, 2004; Ganguly *et al.*, 2008; Casella & Guillotti, 1983). A few structural studies have been performed on Schiff base complexes derived from 2-hydroxyacetophenone and amino acids (Usman *et al.*, 2003; Basu Baul *et al.*, 2007; Parekh *et al.*, 2006). We report here the crystal structure of the title Cu^{II} complex.

The structure consists of discrete monomeric square-planar Cu^{II} complex (Fig. 1 and Table 1). The four basal positions are occupied by three donor atoms from the tridentate Schiff base ligand, which furnishes an ONO donor set, with the fourth position occupied by one N atom from the imidazole ligand. The nitrogen heterocycle is planar and it forms an angle of 14.7 (2)° with the C1—C6 ring.

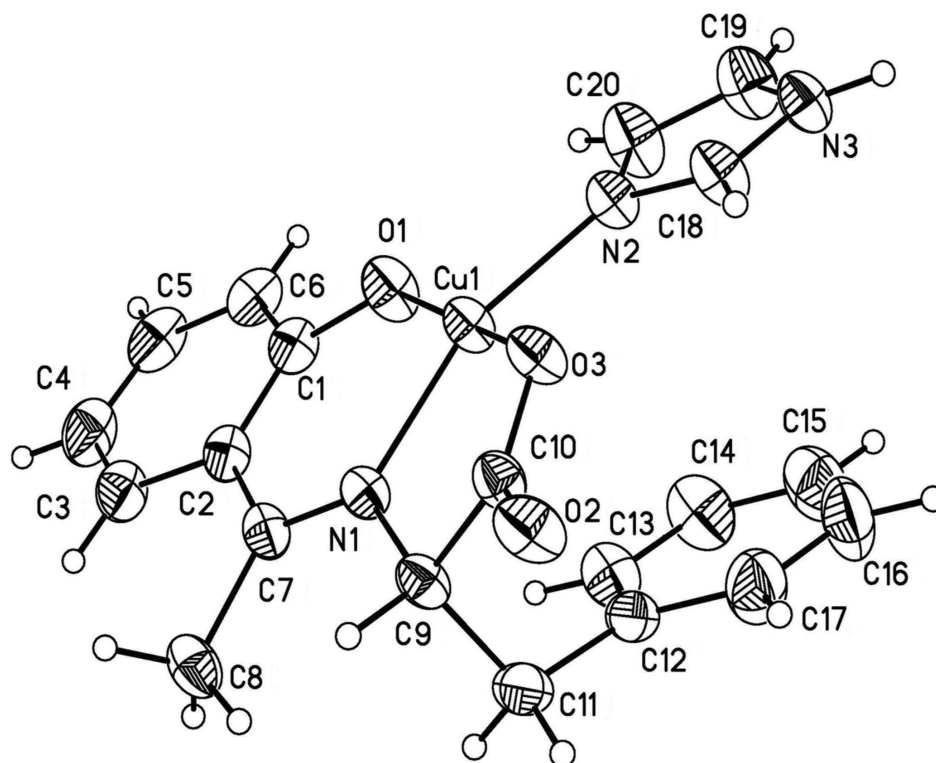
The crystal structure is stabilized by N—H...O type hydrogen bonds (Fig. 2 and Table 2). The H atom attached to N3 is hydrogen-bonded to the neighboring carboxylate oxygen O2 to form a dimer.

S2. Experimental

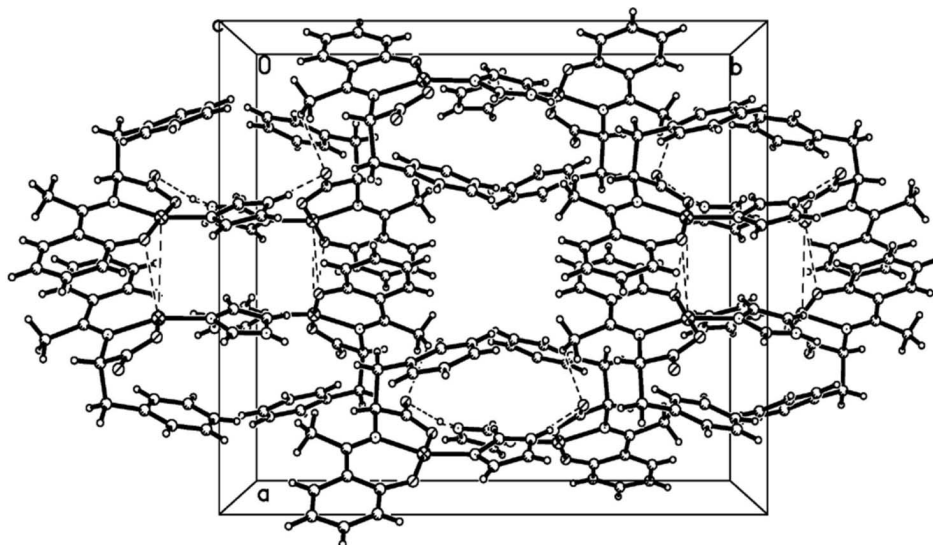
The title compound was synthesized as described in the literature (Plesch *et al.*, 1997). To *L*-phenylalanine (1.00 mmol) and potassium hydroxide (1.00 mmol) in 10 ml of methanol was added 2-hydroxyacetophenone (1.00 mmol in 10 ml of methanol) dropwise. The yellow solution was stirred for 2 h at 333 K. The resultant mixture was added dropwise to copper(II) acetate monohydrate (1.00 mmol) and imidazole (1.00 mmol) in an aqueous methanol solution (20 ml, 1:1 v/v), and heated with stirring for 2 h at 333 K. The dark blue solution was filtered and left for several days; the resulting dark blue crystals were filtered off, washed with water, and dried under vacuum.

S3. Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) or 0.97 Å (CH₂) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, C—H = 0.96 Å (CH₃) and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, and with N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

**Figure 2**

A view of the crystal packing along the *c* axis. Hydrogen bonds are shown as dashed lines.

(1H-Imidazole- κ N³){N-[1-(2-oxidophenyl- κ O)ethylidene]-L-phenylalaninato- κ^2 N,O}copper(II)*Crystal data*[Cu(C₁₇H₁₅NO₃)(C₃H₄N₂)] $M_r = 412.92$ Orthorhombic, $C222_1$

Hall symbol: C 2c 2

 $a = 16.8029$ (16) Å $b = 19.8231$ (19) Å $c = 11.3642$ (11) Å $V = 3785.3$ (6) Å³ $Z = 8$ $F(000) = 1704$ $D_x = 1.449$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3925 reflections

 $\theta = 2.4$ – 23.2° $\mu = 1.18$ mm⁻¹ $T = 291$ K

Block, dark blue

 $0.43 \times 0.34 \times 0.25$ mm*Data collection*Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(*SADABS*; Sheldrick, 1996) $T_{\min} = 0.630$, $T_{\max} = 0.759$

10101 measured reflections

3534 independent reflections

3008 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.027$ $\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.4^\circ$ $h = -20 \rightarrow 16$ $k = -24 \rightarrow 23$ $l = -13 \rightarrow 13$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.067$ $S = 1.01$

3534 reflections

245 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 1.1795P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.21$ e Å⁻³ $\Delta\rho_{\min} = -0.16$ e Å⁻³Absolute structure: Flack (1983), 1557 Friedel
pairsAbsolute structure parameter: -0.029 (12)*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	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.10619 (2)	0.367615 (16)	0.77896 (3)	0.04364 (11)
N1	0.13985 (13)	0.27457 (10)	0.80032 (19)	0.0406 (5)
N2	0.10665 (16)	0.46531 (10)	0.75384 (17)	0.0459 (5)

N3	0.13752 (15)	0.57138 (11)	0.7787 (3)	0.0547 (6)
H3D	0.1544	0.6078	0.8115	0.066*
O1	0.05861 (14)	0.34996 (10)	0.63167 (17)	0.0624 (6)
O2	0.20326 (14)	0.32527 (10)	1.08596 (17)	0.0577 (6)
O3	0.14173 (11)	0.37985 (8)	0.94100 (15)	0.0470 (5)
C1	0.04519 (18)	0.29043 (15)	0.5868 (2)	0.0485 (7)
C2	0.06894 (17)	0.22761 (15)	0.6360 (2)	0.0461 (7)
C3	0.0429 (2)	0.16858 (17)	0.5793 (3)	0.0615 (9)
H3	0.0564	0.1271	0.6117	0.074*
C4	-0.0015 (2)	0.1697 (2)	0.4781 (4)	0.0778 (11)
H4	-0.0192	0.1296	0.4447	0.093*
C5	-0.0197 (2)	0.2304 (2)	0.4260 (3)	0.0704 (10)
H5	-0.0475	0.2312	0.3553	0.084*
C6	0.0028 (2)	0.28950 (16)	0.4780 (3)	0.0585 (8)
H6	-0.0098	0.3301	0.4416	0.070*
C7	0.11970 (16)	0.22199 (12)	0.7394 (2)	0.0444 (7)
C8	0.15118 (19)	0.15280 (12)	0.7715 (3)	0.0580 (8)
H8A	0.1901	0.1570	0.8328	0.087*
H8B	0.1753	0.1325	0.7035	0.087*
H8C	0.1081	0.1250	0.7984	0.087*
C9	0.19625 (17)	0.27141 (13)	0.8989 (2)	0.0454 (7)
H9	0.1897	0.2284	0.9404	0.054*
C10	0.17829 (18)	0.32911 (13)	0.9830 (2)	0.0439 (7)
C11	0.28234 (18)	0.27726 (15)	0.8539 (3)	0.0563 (8)
H11A	0.3185	0.2738	0.9201	0.068*
H11B	0.2933	0.2398	0.8014	0.068*
C12	0.29811 (17)	0.34248 (14)	0.7897 (3)	0.0520 (7)
C13	0.2807 (2)	0.34864 (17)	0.6704 (3)	0.0656 (10)
H13	0.2606	0.3117	0.6296	0.079*
C14	0.2928 (3)	0.4089 (2)	0.6120 (3)	0.0845 (12)
H14	0.2813	0.4122	0.5321	0.101*
C15	0.3216 (3)	0.4640 (2)	0.6713 (4)	0.0921 (13)
H15	0.3292	0.5047	0.6321	0.110*
C16	0.3390 (3)	0.45879 (18)	0.7879 (5)	0.0925 (14)
H16	0.3589	0.4960	0.8281	0.111*
C17	0.3274 (2)	0.39883 (19)	0.8466 (4)	0.0814 (11)
H17	0.3396	0.3962	0.9263	0.098*
C18	0.13541 (19)	0.51078 (14)	0.8262 (3)	0.0560 (9)
H18	0.1524	0.5013	0.9024	0.067*
C19	0.1082 (2)	0.56540 (16)	0.6691 (3)	0.0731 (10)
H19	0.1025	0.5998	0.6140	0.088*
C20	0.0885 (2)	0.49998 (17)	0.6544 (3)	0.0708 (11)
H20	0.0660	0.4816	0.5868	0.085*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0632 (2)	0.03698 (15)	0.03072 (15)	0.00253 (17)	-0.00760 (17)	-0.00122 (14)

N1	0.0497 (13)	0.0383 (11)	0.0339 (13)	0.0008 (10)	0.0026 (10)	-0.0022 (9)
N2	0.0637 (15)	0.0421 (11)	0.0319 (12)	0.0013 (11)	-0.0068 (12)	0.0016 (9)
N3	0.0760 (18)	0.0383 (12)	0.0498 (14)	0.0005 (11)	-0.0040 (14)	0.0027 (12)
O1	0.0910 (16)	0.0539 (14)	0.0424 (11)	-0.0013 (11)	-0.0241 (11)	-0.0035 (10)
O2	0.0849 (16)	0.0513 (12)	0.0368 (10)	0.0122 (11)	-0.0180 (11)	0.0010 (9)
O3	0.0702 (13)	0.0376 (10)	0.0333 (10)	0.0094 (9)	-0.0094 (8)	-0.0010 (8)
C1	0.0508 (18)	0.0605 (19)	0.0342 (15)	-0.0049 (15)	0.0044 (13)	-0.0126 (14)
C2	0.0489 (18)	0.0522 (17)	0.0374 (15)	-0.0067 (14)	0.0086 (13)	-0.0135 (13)
C3	0.062 (2)	0.0598 (19)	0.062 (2)	-0.0079 (16)	0.0073 (17)	-0.0249 (17)
C4	0.070 (2)	0.084 (2)	0.080 (3)	-0.017 (2)	-0.001 (2)	-0.039 (2)
C5	0.057 (2)	0.109 (3)	0.046 (2)	-0.010 (2)	-0.0005 (17)	-0.030 (2)
C6	0.0519 (19)	0.084 (2)	0.0400 (19)	-0.0024 (19)	0.0000 (13)	-0.0078 (18)
C7	0.0538 (18)	0.0392 (13)	0.0400 (16)	-0.0032 (12)	0.0140 (13)	-0.0051 (11)
C8	0.078 (2)	0.0403 (15)	0.0562 (18)	0.0001 (13)	0.0123 (18)	-0.0059 (15)
C9	0.0586 (19)	0.0357 (14)	0.0419 (15)	0.0043 (13)	-0.0051 (14)	0.0034 (12)
C10	0.0550 (19)	0.0377 (15)	0.0391 (15)	-0.0003 (13)	-0.0068 (14)	0.0017 (12)
C11	0.056 (2)	0.0505 (18)	0.063 (2)	0.0117 (15)	-0.0050 (16)	-0.0008 (16)
C12	0.0463 (18)	0.0467 (16)	0.063 (2)	0.0048 (13)	0.0034 (17)	0.0049 (16)
C13	0.082 (3)	0.061 (2)	0.0542 (19)	-0.0013 (17)	0.0195 (18)	-0.0042 (16)
C14	0.115 (3)	0.079 (3)	0.059 (2)	-0.003 (2)	0.022 (2)	0.009 (2)
C15	0.111 (4)	0.065 (3)	0.100 (3)	-0.008 (2)	0.013 (3)	0.018 (2)
C16	0.116 (4)	0.055 (2)	0.107 (4)	-0.026 (2)	-0.029 (3)	0.010 (2)
C17	0.087 (3)	0.073 (2)	0.084 (3)	-0.011 (2)	-0.027 (2)	0.009 (2)
C18	0.088 (3)	0.0427 (16)	0.0375 (16)	0.0023 (15)	-0.0107 (15)	0.0019 (13)
C19	0.108 (3)	0.0540 (19)	0.057 (2)	-0.002 (2)	-0.013 (2)	0.0230 (16)
C20	0.115 (3)	0.0569 (19)	0.0401 (17)	-0.004 (2)	-0.025 (2)	0.0128 (15)

Geometric parameters (Å, °)

Cu1—O1	1.8876 (19)	C7—C8	1.514 (4)
Cu1—N1	1.945 (2)	C8—H8A	0.96
Cu1—O3	1.9511 (18)	C8—H8B	0.96
Cu1—N2	1.958 (2)	C8—H8C	0.96
N1—C7	1.296 (3)	C9—C10	1.520 (4)
N1—C9	1.469 (3)	C9—C11	1.539 (4)
N2—C18	1.312 (4)	C9—H9	0.98
N2—C20	1.358 (4)	C11—C12	1.508 (4)
N3—C18	1.317 (4)	C11—H11A	0.97
N3—C19	1.346 (4)	C11—H11B	0.97
N3—H3D	0.86	C12—C17	1.381 (4)
O1—C1	1.305 (3)	C12—C13	1.392 (4)
O2—C10	1.246 (3)	C13—C14	1.383 (5)
O3—C10	1.271 (3)	C13—H13	0.93
C1—C2	1.422 (4)	C14—C15	1.371 (6)
C1—C6	1.427 (4)	C14—H14	0.93
C2—C3	1.405 (4)	C15—C16	1.361 (6)
C2—C7	1.457 (4)	C15—H15	0.93
C3—C4	1.371 (5)	C16—C17	1.377 (5)

C3—H3	0.93	C16—H16	0.93
C4—C5	1.376 (5)	C17—H17	0.93
C4—H4	0.93	C18—H18	0.93
C5—C6	1.365 (4)	C19—C20	1.349 (4)
C5—H5	0.93	C19—H19	0.93
C6—H6	0.93	C20—H20	0.93
O1—Cu1—N1	93.33 (9)	H8B—C8—H8C	109.5
O1—Cu1—O3	171.74 (9)	N1—C9—C10	108.6 (2)
N1—Cu1—O3	84.90 (8)	N1—C9—C11	110.4 (2)
O1—Cu1—N2	93.20 (9)	C10—C9—C11	109.8 (2)
N1—Cu1—N2	162.84 (10)	N1—C9—H9	109.3
O3—Cu1—N2	90.77 (8)	C10—C9—H9	109.3
C7—N1—C9	122.8 (2)	C11—C9—H9	109.3
C7—N1—Cu1	128.33 (19)	O2—C10—O3	124.3 (3)
C9—N1—Cu1	108.86 (16)	O2—C10—C9	118.5 (2)
C18—N2—C20	104.9 (2)	O3—C10—C9	117.1 (2)
C18—N2—Cu1	126.11 (19)	C12—C11—C9	113.0 (2)
C20—N2—Cu1	128.4 (2)	C12—C11—H11A	109.0
C18—N3—C19	106.8 (3)	C9—C11—H11A	109.0
C18—N3—H3D	126.6	C12—C11—H11B	109.0
C19—N3—H3D	126.6	C9—C11—H11B	109.0
C1—O1—Cu1	125.97 (19)	H11A—C11—H11B	107.8
C10—O3—Cu1	113.79 (16)	C17—C12—C13	117.4 (3)
O1—C1—C2	126.1 (3)	C17—C12—C11	122.0 (3)
O1—C1—C6	115.9 (3)	C13—C12—C11	120.6 (3)
C2—C1—C6	118.0 (3)	C14—C13—C12	120.8 (3)
C3—C2—C1	117.5 (3)	C14—C13—H13	119.6
C3—C2—C7	119.2 (3)	C12—C13—H13	119.6
C1—C2—C7	123.3 (2)	C15—C14—C13	120.2 (4)
C4—C3—C2	122.7 (4)	C15—C14—H14	119.9
C4—C3—H3	118.6	C13—C14—H14	119.9
C2—C3—H3	118.6	C16—C15—C14	119.6 (4)
C3—C4—C5	119.7 (3)	C16—C15—H15	120.2
C3—C4—H4	120.1	C14—C15—H15	120.2
C5—C4—H4	120.1	C15—C16—C17	120.4 (4)
C6—C5—C4	120.2 (3)	C15—C16—H16	119.8
C6—C5—H5	119.9	C17—C16—H16	119.8
C4—C5—H5	119.9	C16—C17—C12	121.5 (4)
C5—C6—C1	121.6 (3)	C16—C17—H17	119.3
C5—C6—H6	119.2	C12—C17—H17	119.3
C1—C6—H6	119.2	N2—C18—N3	112.3 (3)
N1—C7—C2	121.5 (2)	N2—C18—H18	123.9
N1—C7—C8	120.6 (3)	N3—C18—H18	123.9
C2—C7—C8	117.9 (2)	N3—C19—C20	106.8 (3)
C7—C8—H8A	109.5	N3—C19—H19	126.6
C7—C8—H8B	109.5	C20—C19—H19	126.6
H8A—C8—H8B	109.5	C19—C20—N2	109.2 (3)

C7—C8—H8C	109.5	C19—C20—H20	125.4
H8A—C8—H8C	109.5	N2—C20—H20	125.4

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N3—H3D...O2 ⁱ	0.86	1.95	2.789 (3)	166

Symmetry code: (i) $x, -y+1, -z+2$.