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[(*E*)-*N'*-(5-Chloro-2-oxidobenzylidene- κ O)-3,4,5-trimethoxybenzohydrazidato- κ^2 *N',O*](pyridine- κ N)copper(II)

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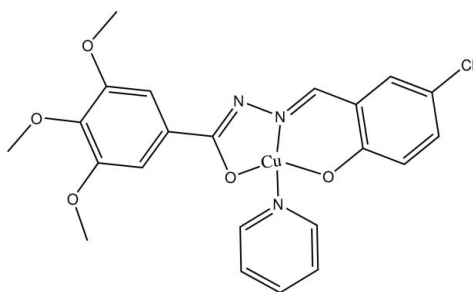
Received 7 March 2011; accepted 16 March 2011

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.031; wR factor = 0.086; data-to-parameter ratio = 13.5.

In the title compound, $[\text{Cu}(\text{C}_{17}\text{H}_{15}\text{ClN}_2\text{O}_5)(\text{C}_5\text{H}_5\text{N})]$, the Cu^{II} atom is coordinated by one N atom and two O atoms from an anionic salicylaldehyde benzoylhydrazone ligand and one pyridine N atom in a distorted square-planar geometry. The bonds displays the usual elongation with mean Cu—O and Cu—N bond lengths of 1.926 and 1.976 Å, respectively. The pyridine ring makes dihedral angles of 26.12 (13) and 11.08 (12)°, respectively, with the trimethoxyphenyl and phenolate rings, which make a dihedral angle of 16.05 (12)° with one another.

Related literature

For the biological activity of salicylaldehyde derivatives, see: Chan *et al.* (1995); Ranford *et al.* (1998); Monfared *et al.* (2009). For related structures, see: Lee *et al.* (2003).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{17}\text{H}_{15}\text{ClN}_2\text{O}_5)(\text{C}_5\text{H}_5\text{N})]$
 $M_r = 505.40$

Monoclinic, $P2_1/n$

$a = 14.274$ (4) Å

$b = 7.5763$ (18) Å

$c = 20.753$ (5) Å

$\beta = 99.108$ (4)°

$V = 2216.1$ (9) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.15$ mm⁻¹

$T = 298$ K

$0.19 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

(*SADABS*; Bruker, 1998)

$T_{\text{min}} = 0.812$, $T_{\text{max}} = 0.875$

11265 measured reflections

3908 independent reflections

3184 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.086$

$S = 1.04$

3908 reflections

289 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.27$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.37$ e Å⁻³

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2271).

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supporting information

Acta Cryst. (2011). E67, m526 [doi:10.1107/S1600536811009901]

[(*E*)-*N'*-(5-Chloro-2-oxidobenzylidene- κ O)-3,4,5-trimethoxybenzohydrazidato- κ^2 N',O](pyridine- κ N)copper(II)

Yu-Min Wang, Xiao-Hui Lin, Zhen Chen, Hong-Li Jiang and Chang-Jun Zhang

S1. Comment

Transition metal complexes with potential biological activity are the focus of extensive investigation. Salicylaldehyde benzoylhydrazone possess mild bacteriostatic activity and inhibits DNA synthesis and cell growth (Chan *et al.*; 1995). Salicylaldehyde acetylhydrazone displays radioprotective properties (Ranford *et al.*; 1998). Because of the biological interest in this type of chelate system, several structural studies have been carried out on copper with their analogues (Lee *et al.*; 2003). The copper(II) complex was shown to be significantly more potent than the metal-free chelate, leading to the suggestion that the metal complex was the biologically active species (Monfared *et al.*; 2009). We report here the crystal structure of the title compound, (I) (Fig. 1). It can be seen that the coordination environment of the copper atom consists of two oxygen atoms and one nitrogen atom from the salicylaldehyde benzoylhydrazone, and one nitrogen atom from the pyridine groups, making up a distorted square-planar environment. The bond length displays the usual elongation: Cu—O = 1.9256 (average) and Cu—N = 1.9755 (average). The pyridine ring makes dihedral angles of 26.12° and 11.08°, respectively, with the C9—C14 and C1—C6 phenyl rings. The C1—C6 benzene ring system makes a dihedral angle of 16.05° with the other C9—C14 benzene ring.

S2. Experimental

Mixture of 20 ml aqueous solution of copper (II) acetate (0.2 mmol) with 2 ml of pyridine was stirred with 20 ml ethanol solution of (*E*)-*N'*-(5-chloro-2-hydroxybenzylidene)-3,4,5-trimethoxybenzohydrazide for 1 h. The resulted solution was leaved in dark place for evaporation. After 1 week of stating blue needle-like shape crystals were grown.

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97 Å (for CH₂ groups) and 0.96 Å (for CH₃ groups), their isotropic displacement parameters were set to 1.2 times (1.5 times for CH₃ groups) the equivalent displacement parameter of their parent atoms.

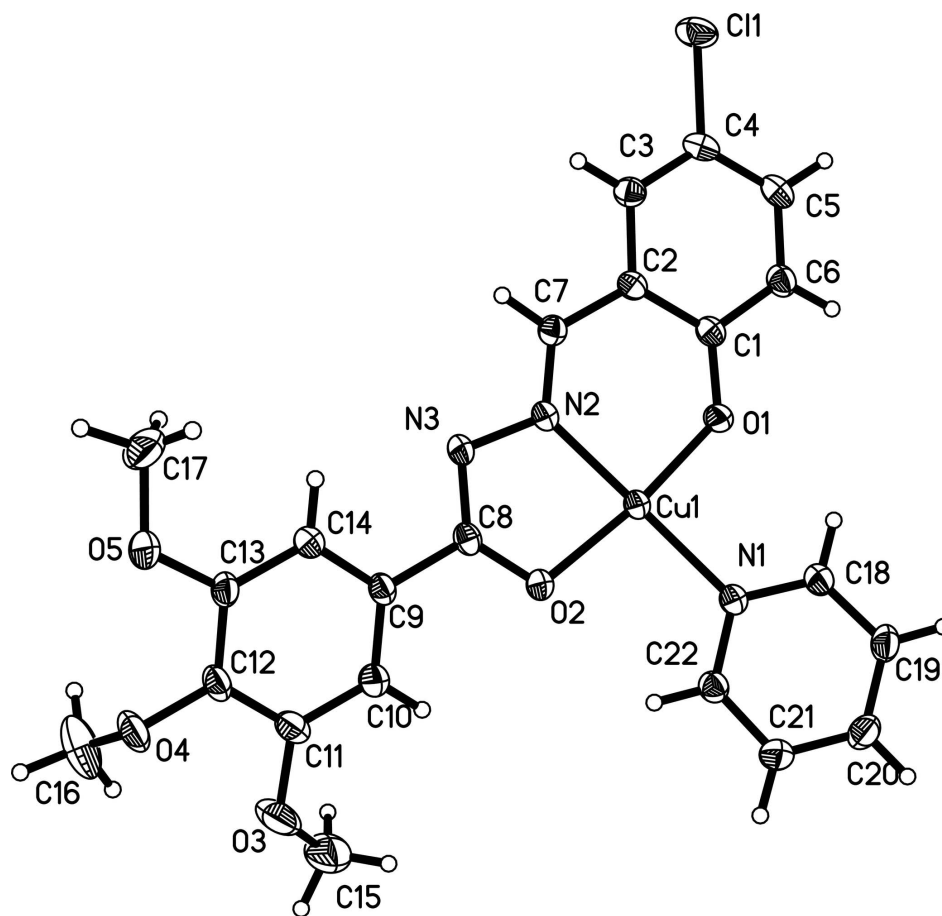


Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

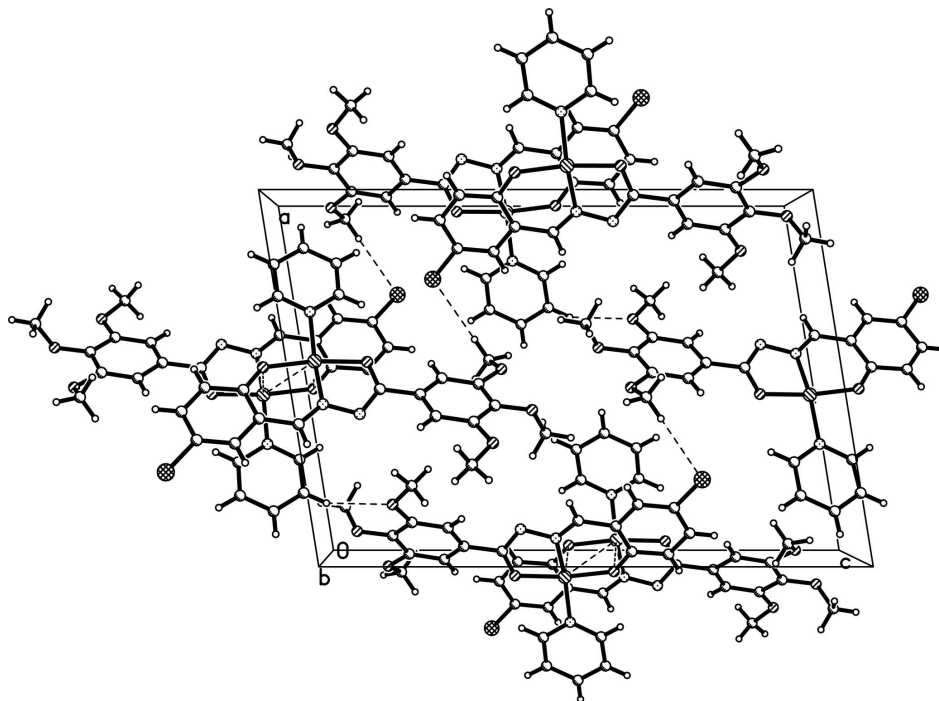


Figure 2

Packing diagram.

[(*E*)-*N'*-(5-Chloro-2-oxidobenzylidene- κ O)-3,4,5-trimethoxybenzohydrazidato- κ^2 N',O](pyridine- κ N)copper(II)

Crystal data[Cu(C₁₇H₁₅ClN₂O₅)(C₅H₅N)] $M_r = 505.40$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 14.274$ (4) Å $b = 7.5763$ (18) Å $c = 20.753$ (5) Å $\beta = 99.108$ (4)° $V = 2216.1$ (9) Å³ $Z = 4$ $F(000) = 1036$ $D_x = 1.515$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3527 reflections

 $\theta = 2.9$ – 25.3 ° $\mu = 1.15$ mm⁻¹ $T = 298$ K

Block, blue

 $0.19 \times 0.16 \times 0.12$ mm*Data collection*Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 1998)

 $T_{\min} = 0.812$, $T_{\max} = 0.875$

11265 measured reflections

3908 independent reflections

3184 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.027$ $\theta_{\text{max}} = 25.0$ °, $\theta_{\text{min}} = 1.6$ ° $h = -15 \rightarrow 17$ $k = -8 \rightarrow 9$ $l = -20 \rightarrow 24$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.086$
 $S = 1.04$
 3908 reflections
 289 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
 $w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.808P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| Cu1 | 0.54442 (2) | 0.14856 (4) | 0.056192 (13) | 0.03244 (11) |
| Cl1 | 0.26557 (6) | 0.62229 (10) | -0.21238 (3) | 0.0569 (2) |
| O1 | 0.52842 (12) | 0.1751 (2) | -0.03651 (8) | 0.0393 (4) |
| O2 | 0.54254 (12) | 0.1224 (2) | 0.14894 (8) | 0.0364 (4) |
| O3 | 0.5244 (2) | -0.0473 (3) | 0.38634 (10) | 0.0825 (8) |
| O4 | 0.41727 (15) | 0.2050 (3) | 0.42842 (8) | 0.0565 (5) |
| O5 | 0.33613 (15) | 0.4566 (3) | 0.34986 (9) | 0.0655 (6) |
| N1 | 0.67522 (14) | 0.0438 (3) | 0.05888 (9) | 0.0324 (4) |
| N2 | 0.43295 (14) | 0.2875 (3) | 0.06254 (9) | 0.0312 (4) |
| N3 | 0.40808 (14) | 0.2968 (3) | 0.12482 (9) | 0.0352 (5) |
| C1 | 0.46948 (17) | 0.2826 (3) | -0.07312 (11) | 0.0337 (5) |
| C2 | 0.39692 (17) | 0.3819 (3) | -0.04970 (11) | 0.0315 (5) |
| C3 | 0.33515 (18) | 0.4867 (3) | -0.09362 (12) | 0.0370 (6) |
| H3 | 0.2878 | 0.5516 | -0.0784 | 0.044* |
| C4 | 0.34372 (18) | 0.4943 (3) | -0.15816 (12) | 0.0386 (6) |
| C5 | 0.4148 (2) | 0.3997 (3) | -0.18158 (12) | 0.0421 (6) |
| H5 | 0.4209 | 0.4063 | -0.2255 | 0.051* |
| C6 | 0.47585 (19) | 0.2969 (3) | -0.13977 (12) | 0.0399 (6) |
| H6 | 0.5231 | 0.2346 | -0.1561 | 0.048* |
| C7 | 0.38229 (18) | 0.3777 (3) | 0.01742 (12) | 0.0346 (6) |
| H7 | 0.3329 | 0.4448 | 0.0289 | 0.042* |
| C8 | 0.47163 (17) | 0.2079 (3) | 0.16524 (11) | 0.0328 (5) |
| C9 | 0.45815 (17) | 0.2063 (3) | 0.23496 (11) | 0.0333 (5) |
| C10 | 0.50005 (19) | 0.0761 (4) | 0.27666 (12) | 0.0423 (6) |
| H10 | 0.5382 | -0.0089 | 0.2615 | 0.051* |

| | | | | |
|------|--------------|-------------|--------------|-------------|
| C11 | 0.4850 (2) | 0.0729 (4) | 0.34094 (12) | 0.0464 (7) |
| C12 | 0.42910 (18) | 0.2013 (4) | 0.36393 (11) | 0.0411 (6) |
| C13 | 0.38825 (18) | 0.3340 (4) | 0.32232 (12) | 0.0410 (6) |
| C14 | 0.40278 (18) | 0.3369 (3) | 0.25749 (12) | 0.0393 (6) |
| H14 | 0.3757 | 0.4253 | 0.2295 | 0.047* |
| C15 | 0.5491 (3) | -0.2135 (5) | 0.36663 (18) | 0.0856 (12) |
| H15A | 0.4979 | -0.2609 | 0.3360 | 0.128* |
| H15B | 0.5616 | -0.2899 | 0.4039 | 0.128* |
| H15C | 0.6049 | -0.2046 | 0.3464 | 0.128* |
| C16 | 0.3549 (3) | 0.0777 (6) | 0.44687 (19) | 0.1005 (15) |
| H16A | 0.2959 | 0.0819 | 0.4174 | 0.151* |
| H16B | 0.3437 | 0.1018 | 0.4904 | 0.151* |
| H16C | 0.3826 | -0.0374 | 0.4454 | 0.151* |
| C17 | 0.2831 (3) | 0.5821 (5) | 0.30812 (17) | 0.0887 (13) |
| H17A | 0.3257 | 0.6550 | 0.2883 | 0.133* |
| H17B | 0.2469 | 0.6545 | 0.3331 | 0.133* |
| H17C | 0.2409 | 0.5216 | 0.2747 | 0.133* |
| C18 | 0.71659 (18) | 0.0346 (4) | 0.00516 (12) | 0.0414 (6) |
| H18 | 0.6856 | 0.0849 | -0.0332 | 0.050* |
| C19 | 0.80282 (19) | -0.0460 (4) | 0.00440 (13) | 0.0497 (7) |
| H19 | 0.8296 | -0.0487 | -0.0336 | 0.060* |
| C20 | 0.8487 (2) | -0.1221 (4) | 0.06053 (14) | 0.0481 (7) |
| H20 | 0.9064 | -0.1793 | 0.0610 | 0.058* |
| C21 | 0.80784 (19) | -0.1126 (4) | 0.11634 (13) | 0.0447 (7) |
| H21 | 0.8378 | -0.1629 | 0.1551 | 0.054* |
| C22 | 0.72216 (18) | -0.0276 (3) | 0.11392 (12) | 0.0368 (6) |
| H22 | 0.6957 | -0.0192 | 0.1520 | 0.044* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Cu1 | 0.03527 (18) | 0.03684 (19) | 0.02615 (17) | 0.00328 (13) | 0.00780 (12) | 0.00003 (12) |
| Cl1 | 0.0675 (5) | 0.0611 (5) | 0.0370 (4) | 0.0104 (4) | -0.0071 (3) | 0.0082 (3) |
| O1 | 0.0453 (11) | 0.0446 (10) | 0.0289 (9) | 0.0119 (8) | 0.0083 (8) | 0.0031 (8) |
| O2 | 0.0374 (10) | 0.0434 (10) | 0.0296 (9) | 0.0054 (8) | 0.0092 (7) | -0.0010 (7) |
| O3 | 0.136 (2) | 0.0742 (16) | 0.0376 (12) | 0.0460 (16) | 0.0132 (13) | 0.0155 (11) |
| O4 | 0.0654 (13) | 0.0796 (14) | 0.0270 (10) | -0.0020 (11) | 0.0151 (9) | 0.0004 (9) |
| O5 | 0.0726 (15) | 0.0912 (16) | 0.0354 (11) | 0.0362 (13) | 0.0167 (10) | -0.0040 (11) |
| N1 | 0.0345 (11) | 0.0330 (11) | 0.0300 (11) | -0.0024 (9) | 0.0065 (9) | -0.0012 (9) |
| N2 | 0.0341 (11) | 0.0341 (11) | 0.0261 (10) | -0.0016 (9) | 0.0071 (8) | 0.0000 (9) |
| N3 | 0.0374 (12) | 0.0442 (12) | 0.0253 (10) | 0.0027 (10) | 0.0088 (9) | 0.0001 (9) |
| C1 | 0.0393 (14) | 0.0309 (13) | 0.0310 (13) | -0.0036 (11) | 0.0061 (10) | -0.0003 (11) |
| C2 | 0.0351 (13) | 0.0283 (13) | 0.0308 (13) | -0.0037 (10) | 0.0044 (10) | 0.0007 (10) |
| C3 | 0.0400 (15) | 0.0337 (13) | 0.0368 (14) | 0.0004 (11) | 0.0043 (11) | 0.0005 (11) |
| C4 | 0.0484 (16) | 0.0319 (13) | 0.0321 (14) | -0.0032 (12) | -0.0038 (11) | 0.0046 (11) |
| C5 | 0.0558 (17) | 0.0419 (15) | 0.0285 (13) | -0.0072 (13) | 0.0063 (12) | 0.0020 (11) |
| C6 | 0.0484 (16) | 0.0393 (14) | 0.0339 (14) | 0.0017 (12) | 0.0125 (12) | -0.0002 (11) |
| C7 | 0.0367 (14) | 0.0347 (13) | 0.0333 (13) | 0.0020 (11) | 0.0083 (11) | -0.0010 (11) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C8 | 0.0365 (14) | 0.0342 (13) | 0.0285 (12) | -0.0069 (11) | 0.0076 (11) | -0.0035 (10) |
| C9 | 0.0328 (13) | 0.0422 (14) | 0.0255 (12) | -0.0041 (11) | 0.0064 (10) | -0.0023 (11) |
| C10 | 0.0471 (16) | 0.0467 (15) | 0.0342 (14) | 0.0078 (13) | 0.0097 (12) | -0.0018 (12) |
| C11 | 0.0548 (18) | 0.0527 (17) | 0.0309 (14) | 0.0034 (14) | 0.0043 (12) | 0.0055 (12) |
| C12 | 0.0426 (15) | 0.0576 (17) | 0.0242 (13) | -0.0049 (13) | 0.0083 (11) | -0.0043 (12) |
| C13 | 0.0369 (14) | 0.0573 (17) | 0.0300 (13) | 0.0056 (12) | 0.0094 (11) | -0.0066 (12) |
| C14 | 0.0403 (15) | 0.0478 (15) | 0.0297 (13) | 0.0050 (12) | 0.0053 (11) | -0.0002 (11) |
| C15 | 0.110 (3) | 0.072 (2) | 0.075 (2) | 0.030 (2) | 0.018 (2) | 0.024 (2) |
| C16 | 0.132 (4) | 0.113 (3) | 0.069 (3) | -0.036 (3) | 0.056 (3) | 0.000 (2) |
| C17 | 0.089 (3) | 0.115 (3) | 0.062 (2) | 0.061 (3) | 0.009 (2) | -0.010 (2) |
| C18 | 0.0392 (15) | 0.0530 (16) | 0.0325 (14) | 0.0007 (12) | 0.0073 (11) | 0.0036 (12) |
| C19 | 0.0411 (16) | 0.071 (2) | 0.0405 (16) | 0.0039 (14) | 0.0158 (12) | -0.0036 (14) |
| C20 | 0.0358 (15) | 0.0576 (18) | 0.0512 (17) | 0.0086 (13) | 0.0082 (13) | -0.0046 (14) |
| C21 | 0.0419 (16) | 0.0521 (17) | 0.0387 (15) | 0.0044 (13) | 0.0016 (12) | 0.0022 (12) |
| C22 | 0.0392 (14) | 0.0402 (14) | 0.0313 (13) | -0.0005 (11) | 0.0065 (11) | -0.0015 (11) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-----------|
| Cu1—O1 | 1.9119 (16) | C7—H7 | 0.9300 |
| Cu1—N2 | 1.930 (2) | C8—C9 | 1.490 (3) |
| Cu1—O2 | 1.9394 (16) | C9—C10 | 1.384 (4) |
| Cu1—N1 | 2.021 (2) | C9—C14 | 1.393 (3) |
| Cl1—C4 | 1.747 (3) | C10—C11 | 1.385 (3) |
| O1—C1 | 1.321 (3) | C10—H10 | 0.9300 |
| O2—C8 | 1.291 (3) | C11—C12 | 1.390 (4) |
| O3—C11 | 1.366 (3) | C12—C13 | 1.392 (4) |
| O3—C15 | 1.386 (4) | C13—C14 | 1.394 (3) |
| O4—C12 | 1.375 (3) | C14—H14 | 0.9300 |
| O4—C16 | 1.406 (4) | C15—H15A | 0.9600 |
| O5—C13 | 1.370 (3) | C15—H15B | 0.9600 |
| O5—C17 | 1.421 (4) | C15—H15C | 0.9600 |
| N1—C22 | 1.343 (3) | C16—H16A | 0.9600 |
| N1—C18 | 1.344 (3) | C16—H16B | 0.9600 |
| N2—C7 | 1.285 (3) | C16—H16C | 0.9600 |
| N2—N3 | 1.395 (2) | C17—H17A | 0.9600 |
| N3—C8 | 1.319 (3) | C17—H17B | 0.9600 |
| C1—C6 | 1.405 (3) | C17—H17C | 0.9600 |
| C1—C2 | 1.426 (3) | C18—C19 | 1.376 (4) |
| C2—C3 | 1.408 (3) | C18—H18 | 0.9300 |
| C2—C7 | 1.441 (3) | C19—C20 | 1.370 (4) |
| C3—C4 | 1.365 (3) | C19—H19 | 0.9300 |
| C3—H3 | 0.9300 | C20—C21 | 1.378 (4) |
| C4—C5 | 1.391 (4) | C20—H20 | 0.9300 |
| C5—C6 | 1.371 (4) | C21—C22 | 1.376 (4) |
| C5—H5 | 0.9300 | C21—H21 | 0.9300 |
| C6—H6 | 0.9300 | C22—H22 | 0.9300 |
| O1—Cu1—N2 | 92.45 (7) | C11—C10—H10 | 120.1 |

| | | | |
|--------------|-------------|---------------|--------------|
| O1—Cu1—O2 | 172.44 (7) | O3—C11—C10 | 124.5 (3) |
| N2—Cu1—O2 | 81.20 (7) | O3—C11—C12 | 115.2 (2) |
| O1—Cu1—N1 | 91.82 (7) | C10—C11—C12 | 120.2 (2) |
| N2—Cu1—N1 | 168.60 (8) | O4—C12—C11 | 120.9 (2) |
| O2—Cu1—N1 | 95.18 (7) | O4—C12—C13 | 119.0 (2) |
| C1—O1—Cu1 | 127.39 (15) | C11—C12—C13 | 120.0 (2) |
| C8—O2—Cu1 | 110.09 (14) | O5—C13—C12 | 115.6 (2) |
| C11—O3—C15 | 119.9 (2) | O5—C13—C14 | 124.4 (2) |
| C12—O4—C16 | 115.6 (2) | C12—C13—C14 | 119.9 (2) |
| C13—O5—C17 | 118.1 (2) | C9—C14—C13 | 119.5 (2) |
| C22—N1—C18 | 117.3 (2) | C9—C14—H14 | 120.3 |
| C22—N1—Cu1 | 121.05 (16) | C13—C14—H14 | 120.3 |
| C18—N1—Cu1 | 121.52 (17) | O3—C15—H15A | 109.5 |
| C7—N2—N3 | 116.9 (2) | O3—C15—H15B | 109.5 |
| C7—N2—Cu1 | 127.97 (16) | H15A—C15—H15B | 109.5 |
| N3—N2—Cu1 | 115.09 (14) | O3—C15—H15C | 109.5 |
| C8—N3—N2 | 108.26 (19) | H15A—C15—H15C | 109.5 |
| O1—C1—C6 | 118.6 (2) | H15B—C15—H15C | 109.5 |
| O1—C1—C2 | 124.0 (2) | O4—C16—H16A | 109.5 |
| C6—C1—C2 | 117.3 (2) | O4—C16—H16B | 109.5 |
| C3—C2—C1 | 119.4 (2) | H16A—C16—H16B | 109.5 |
| C3—C2—C7 | 117.8 (2) | O4—C16—H16C | 109.5 |
| C1—C2—C7 | 122.8 (2) | H16A—C16—H16C | 109.5 |
| C4—C3—C2 | 121.0 (2) | H16B—C16—H16C | 109.5 |
| C4—C3—H3 | 119.5 | O5—C17—H17A | 109.5 |
| C2—C3—H3 | 119.5 | O5—C17—H17B | 109.5 |
| C3—C4—C5 | 120.3 (2) | H17A—C17—H17B | 109.5 |
| C3—C4—C11 | 120.5 (2) | O5—C17—H17C | 109.5 |
| C5—C4—C11 | 119.17 (19) | H17A—C17—H17C | 109.5 |
| C6—C5—C4 | 119.8 (2) | H17B—C17—H17C | 109.5 |
| C6—C5—H5 | 120.1 | N1—C18—C19 | 122.9 (2) |
| C4—C5—H5 | 120.1 | N1—C18—H18 | 118.5 |
| C5—C6—C1 | 122.2 (2) | C19—C18—H18 | 118.5 |
| C5—C6—H6 | 118.9 | C20—C19—C18 | 119.0 (2) |
| C1—C6—H6 | 118.9 | C20—C19—H19 | 120.5 |
| N2—C7—C2 | 124.4 (2) | C18—C19—H19 | 120.5 |
| N2—C7—H7 | 117.8 | C19—C20—C21 | 119.0 (3) |
| C2—C7—H7 | 117.8 | C19—C20—H20 | 120.5 |
| O2—C8—N3 | 125.3 (2) | C21—C20—H20 | 120.5 |
| O2—C8—C9 | 118.5 (2) | C22—C21—C20 | 119.0 (2) |
| N3—C8—C9 | 116.1 (2) | C22—C21—H21 | 120.5 |
| C10—C9—C14 | 120.6 (2) | C20—C21—H21 | 120.5 |
| C10—C9—C8 | 120.2 (2) | N1—C22—C21 | 122.7 (2) |
| C14—C9—C8 | 119.2 (2) | N1—C22—H22 | 118.6 |
| C9—C10—C11 | 119.8 (2) | C21—C22—H22 | 118.6 |
| C9—C10—H10 | 120.1 | | |
| N2—Cu1—O1—C1 | 10.7 (2) | Cu1—O2—C8—C9 | -179.27 (16) |

| | | | |
|---------------|--------------|-----------------|-------------|
| N1—Cu1—O1—C1 | -158.7 (2) | N2—N3—C8—O2 | -2.2 (3) |
| N2—Cu1—O2—C8 | -0.24 (15) | N2—N3—C8—C9 | 178.60 (19) |
| N1—Cu1—O2—C8 | 168.87 (15) | O2—C8—C9—C10 | -20.0 (3) |
| O1—Cu1—N1—C22 | -171.09 (18) | N3—C8—C9—C10 | 159.3 (2) |
| N2—Cu1—N1—C22 | 76.9 (4) | O2—C8—C9—C14 | 160.2 (2) |
| O2—Cu1—N1—C22 | 6.06 (19) | N3—C8—C9—C14 | -20.5 (3) |
| O1—Cu1—N1—C18 | 5.5 (2) | C14—C9—C10—C11 | 1.6 (4) |
| N2—Cu1—N1—C18 | -106.5 (4) | C8—C9—C10—C11 | -178.2 (2) |
| O2—Cu1—N1—C18 | -177.36 (19) | C15—O3—C11—C10 | -27.1 (5) |
| O1—Cu1—N2—C7 | -8.4 (2) | C15—O3—C11—C12 | 155.1 (3) |
| O2—Cu1—N2—C7 | 175.7 (2) | C9—C10—C11—O3 | -178.7 (3) |
| N1—Cu1—N2—C7 | 103.5 (4) | C9—C10—C11—C12 | -0.9 (4) |
| O1—Cu1—N2—N3 | 175.03 (16) | C16—O4—C12—C11 | -76.1 (4) |
| O2—Cu1—N2—N3 | -0.85 (15) | C16—O4—C12—C13 | 107.2 (3) |
| N1—Cu1—N2—N3 | -73.0 (4) | O3—C11—C12—O4 | 1.2 (4) |
| C7—N2—N3—C8 | -175.3 (2) | C10—C11—C12—O4 | -176.8 (2) |
| Cu1—N2—N3—C8 | 1.7 (2) | O3—C11—C12—C13 | 177.8 (3) |
| Cu1—O1—C1—C6 | 172.93 (17) | C10—C11—C12—C13 | -0.2 (4) |
| Cu1—O1—C1—C2 | -9.2 (3) | C17—O5—C13—C12 | -172.3 (3) |
| O1—C1—C2—C3 | -177.2 (2) | C17—O5—C13—C14 | 8.6 (4) |
| C6—C1—C2—C3 | 0.7 (3) | O4—C12—C13—O5 | -1.9 (4) |
| O1—C1—C2—C7 | 1.6 (4) | C11—C12—C13—O5 | -178.6 (3) |
| C6—C1—C2—C7 | 179.5 (2) | O4—C12—C13—C14 | 177.3 (2) |
| C1—C2—C3—C4 | 0.1 (4) | C11—C12—C13—C14 | 0.6 (4) |
| C7—C2—C3—C4 | -178.8 (2) | C10—C9—C14—C13 | -1.2 (4) |
| C2—C3—C4—C5 | -0.8 (4) | C8—C9—C14—C13 | 178.7 (2) |
| C2—C3—C4—C11 | 179.08 (18) | O5—C13—C14—C9 | 179.2 (3) |
| C3—C4—C5—C6 | 0.7 (4) | C12—C13—C14—C9 | 0.1 (4) |
| C11—C4—C5—C6 | -179.1 (2) | C22—N1—C18—C19 | 1.0 (4) |
| C4—C5—C6—C1 | 0.1 (4) | Cu1—N1—C18—C19 | -175.7 (2) |
| O1—C1—C6—C5 | 177.2 (2) | N1—C18—C19—C20 | 0.7 (4) |
| C2—C1—C6—C5 | -0.8 (4) | C18—C19—C20—C21 | -1.2 (4) |
| N3—N2—C7—C2 | -179.1 (2) | C19—C20—C21—C22 | 0.3 (4) |
| Cu1—N2—C7—C2 | 4.4 (4) | C18—N1—C22—C21 | -2.0 (4) |
| C3—C2—C7—N2 | 179.7 (2) | Cu1—N1—C22—C21 | 174.66 (19) |
| C1—C2—C7—N2 | 0.9 (4) | C20—C21—C22—N1 | 1.5 (4) |
| Cu1—O2—C8—N3 | 1.5 (3) | | |
