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(2,2′-Bipyridine-κ^2N,N')(3,5-dinitrosalicylato-κ^2O^1,O^2)(pyridine-κN)copper(II)

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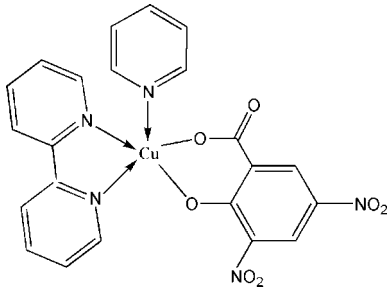
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.052; wR factor = 0.149; data-to-parameter ratio = 12.1.

In the title compound, $[Cu(C_7H_2N_2O_7)(C_5H_5N)(C_{10}H_8N_2)]$, the Cu^{II} atom is coordinated by two O atoms from a 3,5-dinitrosalicylate ligand, two N atoms from a 2,2′-bipyridine ligand and one N atom from a pyridine ligand in a square-pyramidal geometry. The structure is stabilized by C—H···O hydrogen bonds and π–π interactions between the bipyridine ligands, with a centroid–centroid distance between neighbouring aromatic rings of 3.96 (8) Å.

Related literature

For related literature, see: He *et al.* (2005, 2006); Lemoine *et al.* (2004); Thurston *et al.* (2004); Valigura *et al.* (2004); Wang & Okabe (2004); Wen *et al.* (2007); Zhu *et al.* (2003).



Experimental

Crystal data

$[Cu(C_7H_2N_2O_7)(C_5H_5N)(C_{10}H_8N_2)]$
M_r = 524.93
Triclinic, $P\overline{1}$
a = 9.981 (2) Å
b = 10.269 (2) Å
c = 11.913 (2) Å
α = 68.99 (3)°
β = 67.88 (3)°
γ = 79.08 (3)°
V = 1053.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 (2) K
0.24 × 0.23 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.767, T_{max} = 0.797
8700 measured reflections
3813 independent reflections
3149 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.149
S = 1.10
3813 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.896 (3)	Cu1—N3	2.020 (3)
Cu1—O3	1.917 (3)	Cu1—N5	2.267 (4)
Cu1—N4	2.007 (3)		
O2—Cu1—O3	94.21 (12)	N4—Cu1—N3	80.41 (15)
O2—Cu1—N4	163.41 (15)	O2—Cu1—N5	99.04 (15)
O3—Cu1—N4	90.62 (14)	O3—Cu1—N5	95.26 (13)
O2—Cu1—N3	91.20 (13)	N4—Cu1—N5	96.30 (14)
O3—Cu1—N3	164.71 (15)	N3—Cu1—N5	98.00 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···O1^{i}	0.93	2.31	3.226 (6)	169
C22—H22A···O1^{ii}	0.93	2.47	3.174 (6)	133
C9—H9A···O6^{iii}	0.93	2.68	3.306 (6)	125
C19—H19A···O5^{iv}	0.93	2.64	3.283 (6)	126

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y-1, z+1$; (iv) $-x+2, -y+2, -z+1$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: HY2074).

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supplementary materials

Acta Cryst. (2007). E**63**, m2362-m2363 [**doi:10.1107/S1600536807039876**]

(2,2'-Bipyridine-κ^2N,N')(3,5-dinitrosalicylato-κ^2O^1,O^2)(pyridine-κN)copper(II)

D.-C. Wen, L.-H. Wu, C.-L. Zhong, T.-Y. Xie and H.-G. Ta

Comment

Salicylic acid and its substituted derivatives continue to attract attention because of their versatile coordination modes (Thurston *et al.*, 2004; Valigura *et al.*, 2004; Wang & Okabe, 2004; Zhu *et al.*, 2003) and biological applications (Lemoine *et al.*, 2004). We report here the structure of a Cu^{II} complex with 3,5-dinitrosalicylic acid (He *et al.*, 2005; He *et al.*, 2006; Wen *et al.*, 2007).

In the title complex, the Cu^{II} atom is bonded to two N atoms from a 2,2'-bipyridine ligand, one carboxylate O atom and one phenolato O atom from a 3,5-dinitrosalicylate ligand (Fig. 1). The coordination of the Cu^{II} atom is completed by bonding to a pyridine N atom in the axial direction, giving a square-pyramidal geometry (Table 1). The dihedral angle of the carboxylate group and the aromatic ring in 3,5-dinitrosalicylate ligand is 10.8 (9)°. The two rings in the 2,2'-bipyridine ligand are a little twisted relative to each other, with a dihedral angle of 2.2 (3)°. The adjacent mononuclear units are further connected to each other by C—H···O hydrogen bonds between the 2,2'-bipyridine (or pyridine) ligands and the O atoms from carboxylate and NO_2 groups of the 3,5-dinitrosalicylate ligands (Table 2), resulting in an extended three-dimensional structure (Fig. 2). The partially overlapped arrangement indicates π–π interactions between the approximately parallel 2,2'-bipyridine ligands (the contact distances: $C12\cdots C17^{v}$ = 3.45 (7), $C11\cdots C13^{v}$ = 3.55 (6), $C10\cdots C14^{v}$ = 3.55 (7) Å; symmetry code: (v) $1-x$, $1-y$, $2-z$). The centroid–centroid distance of aromatic rings of the neighboring 2,2'-bipyridine ligands is 3.96 (8) Å. The crystal structure is stabilized by C—H···O hydrogen bonds and π–π interactions.

Experimental

A mixture of $Cu(NO_3)_2{\cdot}4H_2O$ (0.026 g, 0.1 mmol), 2,2'-bipyridine (0.016 g, 0.1 mmol), 3,5-dinitrosalicylic acid (0.046 g, 0.2 mmol), pyridine (0.1 ml), NaOH (0.008 g, 0.2 mmol) and distilled water (10 ml) was put into a 20 ml Teflon-lined autoclave and then heated at 393 K for 48 h. Green block-like crystals of the title compound suitable for X-ray analysis were collected from the reaction mixture.

Refinement

H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

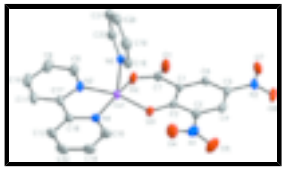

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

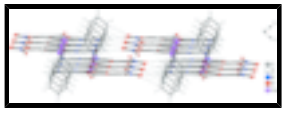

Fig. 2. Packing diagram of the title compound viewed down the *c* axis. Hydrogen bonds are denoted by dashed lines.

(2,2'-Bipyridine-κ^2*N*,*N*')(3,5-dinitrosalicylato-κ^2*O*^{1},*O*^{2})(pyridine- κ*N*)copper(II)

Crystal data

$[Cu(C_7H_2N_2O_7)(C_5H_5N)(C_{10}H_8N_2)]$	$Z = 2$
$M_r = 524.93$	$F_{000} = 534$
Triclinic, $P\overline{1}$	$D_x = 1.654$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.981$ (2) Å	Cell parameters from 3813 reflections
$b = 10.269$ (2) Å	$\theta = 1.9$–25.5°
$c = 11.913$ (2) Å	$\mu = 1.10$ mm^{-1}
$\alpha = 68.99$ (3)°	$T = 293$ (2) K
$\beta = 67.88$ (3)°	Block, green
$\gamma = 79.08$ (3)°	0.24 × 0.23 × 0.21 mm
$V = 1053.9$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	3813 independent reflections
Radiation source: fine-focus sealed tube	3149 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 293$(2) K	$\theta_{max} = 25.5^\circ$
ω scans	$\theta_{min} = 1.9^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 11$
$T_{min} = 0.767$, $T_{max} = 0.797$	$k = -12 \rightarrow 0$
8700 measured reflections	$l = -14 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 1.3696P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
3813 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.73644 (5)	0.53558 (5)	0.63796 (4)	0.03526 (19)
N1	1.1054 (5)	0.8518 (4)	0.4277 (5)	0.0568 (11)
N2	1.1139 (4)	0.8782 (4)	0.0098 (4)	0.0487 (10)
N3	0.5974 (4)	0.3880 (4)	0.7647 (3)	0.0398 (8)
N4	0.7636 (4)	0.5261 (4)	0.7993 (3)	0.0383 (8)
N5	0.5748 (4)	0.7234 (4)	0.6310 (3)	0.0392 (8)
O1	0.7897 (4)	0.4980 (4)	0.2997 (3)	0.0675 (12)
O2	0.7302 (3)	0.4896 (3)	0.4995 (3)	0.0474 (8)
O3	0.9040 (3)	0.6421 (3)	0.5376 (3)	0.0423 (7)
O4	1.0337 (5)	0.8415 (4)	0.5388 (4)	0.0742 (12)
O5	1.2219 (5)	0.9046 (5)	0.3731 (5)	0.0922 (15)
O6	1.2102 (4)	0.9586 (4)	−0.0363 (4)	0.0721 (12)
O7	1.0631 (4)	0.8460 (4)	−0.0548 (3)	0.0661 (10)
C1	0.9028 (4)	0.6550 (4)	0.3326 (4)	0.0316 (8)
C2	0.9467 (4)	0.6966 (4)	0.4161 (4)	0.0343 (9)
C3	1.0503 (4)	0.8015 (5)	0.3536 (4)	0.0398 (10)
C4	1.1040 (5)	0.8609 (5)	0.2222 (5)	0.0458 (11)
H4A	1.1713	0.9288	0.1848	0.055*
C5	1.0565 (5)	0.8179 (4)	0.1485 (4)	0.0398 (10)
C6	0.9573 (4)	0.7168 (4)	0.2024 (4)	0.0380 (9)
H6A	0.9267	0.6899	0.1498	0.046*
C7	0.8009 (5)	0.5402 (5)	0.3796 (4)	0.0383 (9)
C8	0.5166 (5)	0.3232 (5)	0.7363 (5)	0.0474 (11)
H8A	0.5211	0.3478	0.6519	0.057*
C9	0.4261 (6)	0.2202 (5)	0.8288 (5)	0.0589 (14)
H9A	0.3690	0.1776	0.8073	0.071*
C10	0.4227 (6)	0.1824 (5)	0.9525 (5)	0.0620 (15)
H10A	0.3635	0.1131	1.0158	0.074*
C11	0.5064 (6)	0.2467 (5)	0.9828 (5)	0.0554 (13)
H11A	0.5056	0.2204	1.0663	0.066*
C12	0.6925 (5)	0.4151 (6)	1.0246 (4)	0.0531 (12)
H12A	0.6369	0.3507	1.0977	0.064*
C13	0.7826 (6)	0.4939 (6)	1.0325 (5)	0.0614 (15)
H13A	0.7900	0.4832	1.1109	0.074*
C14	0.8622 (6)	0.5890 (6)	0.9233 (5)	0.0575 (13)
H14A	0.9236	0.6439	0.9271	0.069*
C15	0.8506 (5)	0.6029 (5)	0.8071 (5)	0.0480 (11)
H15A	0.9049	0.6673	0.7332	0.058*
C16	0.6849 (5)	0.4322 (5)	0.9066 (4)	0.0404 (10)
C17	0.5929 (5)	0.3521 (4)	0.8872 (4)	0.0412 (10)
C18	0.5984 (5)	0.8385 (5)	0.6463 (4)	0.0448 (11)
H18A	0.6903	0.8471	0.6448	0.054*
C19	0.4958 (6)	0.9440 (5)	0.6640 (5)	0.0536 (12)
H19A	0.5174	1.0221	0.6747	0.064*
C20	0.3603 (6)	0.9338 (6)	0.6658 (5)	0.0596 (14)

H20A	0.2879	1.0038	0.6796	0.072*
C21	0.3327 (5)	0.8176 (6)	0.6469 (5)	0.0575 (14)
H21A	0.2421	0.8083	0.6463	0.069*
C22	0.4424 (5)	0.7168 (5)	0.6292 (4)	0.0468 (11)
H22A	0.4245	0.6394	0.6151	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0393 (3)	0.0428 (3)	0.0239 (3)	−0.0148 (2)	−0.0062 (2)	−0.0092 (2)
N1	0.054 (3)	0.053 (3)	0.074 (3)	−0.022 (2)	−0.024 (2)	−0.020 (2)
N2	0.045 (2)	0.041 (2)	0.036 (2)	0.0020 (17)	−0.0007 (18)	0.0001 (17)
N3	0.046 (2)	0.0372 (19)	0.0293 (17)	−0.0084 (16)	−0.0018 (15)	−0.0104 (15)
N4	0.0372 (18)	0.049 (2)	0.0327 (17)	−0.0015 (15)	−0.0127 (15)	−0.0175 (16)
N5	0.044 (2)	0.042 (2)	0.0341 (18)	−0.0130 (16)	−0.0160 (16)	−0.0069 (15)
O1	0.086 (3)	0.095 (3)	0.0326 (17)	−0.057 (2)	−0.0099 (17)	−0.0172 (17)
O2	0.0548 (19)	0.063 (2)	0.0282 (14)	−0.0365 (16)	−0.0002 (14)	−0.0169 (14)
O3	0.0400 (16)	0.0597 (19)	0.0293 (14)	−0.0219 (14)	−0.0053 (12)	−0.0140 (13)
O4	0.098 (3)	0.084 (3)	0.058 (2)	−0.044 (2)	−0.024 (2)	−0.025 (2)
O5	0.067 (3)	0.121 (4)	0.105 (3)	−0.055 (3)	−0.013 (3)	−0.046 (3)
O6	0.064 (2)	0.062 (2)	0.053 (2)	−0.0251 (19)	0.0093 (19)	0.0038 (18)
O7	0.071 (2)	0.074 (3)	0.0321 (17)	−0.006 (2)	−0.0065 (17)	−0.0024 (17)
C1	0.0288 (19)	0.037 (2)	0.0275 (18)	−0.0069 (16)	−0.0070 (16)	−0.0091 (16)
C2	0.0273 (19)	0.038 (2)	0.037 (2)	−0.0056 (16)	−0.0066 (16)	−0.0129 (17)
C3	0.035 (2)	0.041 (2)	0.049 (2)	−0.0097 (18)	−0.0141 (19)	−0.0166 (19)
C4	0.034 (2)	0.036 (2)	0.052 (3)	−0.0099 (18)	−0.003 (2)	−0.004 (2)
C5	0.035 (2)	0.034 (2)	0.034 (2)	−0.0043 (17)	−0.0023 (17)	−0.0015 (17)
C6	0.038 (2)	0.043 (2)	0.0294 (19)	−0.0043 (18)	−0.0105 (17)	−0.0073 (17)
C7	0.040 (2)	0.051 (3)	0.0290 (19)	−0.0168 (19)	−0.0113 (18)	−0.0123 (18)
C8	0.051 (3)	0.044 (3)	0.044 (2)	−0.018 (2)	−0.003 (2)	−0.015 (2)
C9	0.058 (3)	0.048 (3)	0.064 (3)	−0.017 (2)	−0.001 (3)	−0.024 (2)
C10	0.062 (3)	0.044 (3)	0.057 (3)	−0.020 (2)	0.003 (3)	−0.006 (2)
C11	0.061 (3)	0.045 (3)	0.035 (2)	−0.001 (2)	−0.003 (2)	0.001 (2)
C12	0.052 (3)	0.069 (3)	0.030 (2)	0.011 (2)	−0.014 (2)	−0.014 (2)
C13	0.065 (3)	0.089 (4)	0.034 (2)	0.020 (3)	−0.025 (2)	−0.027 (3)
C14	0.051 (3)	0.084 (4)	0.057 (3)	0.009 (3)	−0.030 (3)	−0.038 (3)
C15	0.047 (3)	0.062 (3)	0.042 (2)	0.001 (2)	−0.020 (2)	−0.021 (2)
C16	0.039 (2)	0.045 (2)	0.028 (2)	0.0075 (19)	−0.0083 (18)	−0.0098 (18)
C17	0.042 (2)	0.036 (2)	0.031 (2)	0.0048 (18)	−0.0031 (18)	−0.0070 (17)
C18	0.048 (3)	0.047 (3)	0.042 (2)	−0.019 (2)	−0.013 (2)	−0.011 (2)
C19	0.066 (3)	0.046 (3)	0.048 (3)	−0.007 (2)	−0.012 (2)	−0.020 (2)
C20	0.058 (3)	0.063 (3)	0.042 (3)	0.005 (3)	−0.011 (2)	−0.010 (2)
C21	0.040 (3)	0.077 (4)	0.047 (3)	−0.016 (3)	−0.016 (2)	−0.002 (3)
C22	0.048 (3)	0.052 (3)	0.043 (2)	−0.016 (2)	−0.018 (2)	−0.009 (2)

Geometric parameters (Å, °)

Cu1—O2	1.896 (3)	C6—H6A	0.9300
Cu1—O3	1.917 (3)	C8—C9	1.388 (6)

Cu1—N4	2.007 (3)	C8—H8A	0.9300
Cu1—N3	2.020 (3)	C9—C10	1.372 (8)
Cu1—N5	2.267 (4)	C9—H9A	0.9300
N1—O5	1.220 (5)	C10—C11	1.367 (8)
N1—O4	1.220 (6)	C10—H10A	0.9300
N1—C3	1.466 (6)	C11—C17	1.394 (6)
N2—O6	1.219 (5)	C11—H11A	0.9300
N2—O7	1.224 (6)	C12—C13	1.367 (8)
N2—C5	1.460 (5)	C12—C16	1.382 (6)
N3—C8	1.334 (6)	C12—H12A	0.9300
N3—C17	1.356 (6)	C13—C14	1.372 (8)
N4—C15	1.326 (6)	C13—H13A	0.9300
N4—C16	1.352 (6)	C14—C15	1.386 (6)
N5—C18	1.334 (6)	C14—H14A	0.9300
N5—C22	1.344 (6)	C15—H15A	0.9300
O1—C7	1.225 (5)	C16—C17	1.468 (6)
O2—C7	1.287 (5)	C18—C19	1.360 (7)
O3—C2	1.278 (5)	C18—H18A	0.9300
C1—C6	1.376 (5)	C19—C20	1.367 (8)
C1—C2	1.439 (6)	C19—H19A	0.9300
C1—C7	1.513 (5)	C20—C21	1.384 (8)
C2—C3	1.432 (5)	C20—H20A	0.9300
C3—C4	1.385 (6)	C21—C22	1.366 (7)
C4—C5	1.364 (7)	C21—H21A	0.9300
C4—H4A	0.9300	C22—H22A	0.9300
C5—C6	1.379 (6)		
O2—Cu1—O3	94.21 (12)	O2—C7—C1	120.4 (3)
O2—Cu1—N4	163.41 (15)	N3—C8—C9	122.0 (5)
O3—Cu1—N4	90.62 (14)	N3—C8—H8A	119.0
O2—Cu1—N3	91.20 (13)	C9—C8—H8A	119.0
O3—Cu1—N3	164.71 (15)	C10—C9—C8	118.6 (5)
N4—Cu1—N3	80.41 (15)	C10—C9—H9A	120.7
O2—Cu1—N5	99.04 (15)	C8—C9—H9A	120.7
O3—Cu1—N5	95.26 (13)	C11—C10—C9	120.1 (5)
N4—Cu1—N5	96.30 (14)	C11—C10—H10A	120.0
N3—Cu1—N5	98.00 (14)	C9—C10—H10A	120.0
O5—N1—O4	123.0 (5)	C10—C11—C17	119.3 (5)
O5—N1—C3	117.2 (5)	C10—C11—H11A	120.3
O4—N1—C3	119.7 (4)	C17—C11—H11A	120.3
O6—N2—O7	123.1 (4)	C13—C12—C16	119.1 (5)
O6—N2—C5	118.3 (5)	C13—C12—H12A	120.4
O7—N2—C5	118.6 (4)	C16—C12—H12A	120.4
C8—N3—C17	119.5 (4)	C12—C13—C14	119.2 (5)
C8—N3—Cu1	125.5 (3)	C12—C13—H13A	120.4
C17—N3—Cu1	114.9 (3)	C14—C13—H13A	120.4
C15—N4—C16	119.4 (4)	C13—C14—C15	119.6 (5)
C15—N4—Cu1	125.4 (3)	C13—C14—H14A	120.2
C16—N4—Cu1	115.2 (3)	C15—C14—H14A	120.2
C18—N5—C22	116.5 (4)	N4—C15—C14	121.3 (5)

C18—N5—Cu1	121.6 (3)	N4—C15—H15A	119.4
C22—N5—Cu1	121.3 (3)	C14—C15—H15A	119.4
C7—O2—Cu1	128.7 (3)	N4—C16—C12	121.4 (4)
C2—O3—Cu1	125.1 (3)	N4—C16—C17	115.0 (4)
C6—C1—C2	120.3 (4)	C12—C16—C17	123.6 (4)
C6—C1—C7	116.3 (4)	N3—C17—C11	120.5 (5)
C2—C1—C7	123.3 (3)	N3—C17—C16	114.4 (4)
O3—C2—C3	120.5 (4)	C11—C17—C16	125.1 (4)
O3—C2—C1	124.2 (4)	N5—C18—C19	123.6 (4)
C3—C2—C1	115.3 (4)	N5—C18—H18A	118.2
C4—C3—C2	123.0 (4)	C19—C18—H18A	118.2
C4—C3—N1	116.3 (4)	C18—C19—C20	119.1 (5)
C2—C3—N1	120.7 (4)	C18—C19—H19A	120.5
C5—C4—C3	118.7 (4)	C20—C19—H19A	120.5
C5—C4—H4A	120.6	C19—C20—C21	118.9 (5)
C3—C4—H4A	120.6	C19—C20—H20A	120.5
C4—C5—C6	121.3 (4)	C21—C20—H20A	120.5
C4—C5—N2	119.3 (4)	C22—C21—C20	118.1 (5)
C6—C5—N2	119.4 (4)	C22—C21—H21A	121.0
C1—C6—C5	121.3 (4)	C20—C21—H21A	121.0
C1—C6—H6A	119.3	N5—C22—C21	123.7 (5)
C5—C6—H6A	119.3	N5—C22—H22A	118.2
O1—C7—O2	122.1 (4)	C21—C22—H22A	118.2
O1—C7—C1	117.5 (4)		
O2—Cu1—N3—C8	−14.4 (4)	C3—C4—C5—N2	−179.1 (4)
O3—Cu1—N3—C8	−125.2 (5)	O6—N2—C5—C4	4.9 (6)
N4—Cu1—N3—C8	−180.0 (4)	O7—N2—C5—C4	−175.0 (4)
N5—Cu1—N3—C8	84.9 (4)	O6—N2—C5—C6	−173.9 (4)
O2—Cu1—N3—C17	163.5 (3)	O7—N2—C5—C6	6.1 (6)
O3—Cu1—N3—C17	52.7 (6)	C2—C1—C6—C5	1.1 (6)
N4—Cu1—N3—C17	−2.2 (3)	C7—C1—C6—C5	−176.9 (4)
N5—Cu1—N3—C17	−97.2 (3)	C4—C5—C6—C1	−0.2 (7)
O2—Cu1—N4—C15	120.4 (5)	N2—C5—C6—C1	178.6 (4)
O3—Cu1—N4—C15	13.3 (4)	Cu1—O2—C7—O1	177.8 (4)
N3—Cu1—N4—C15	−179.1 (4)	Cu1—O2—C7—C1	−1.7 (7)
N5—Cu1—N4—C15	−82.1 (4)	C6—C1—C7—O1	9.6 (6)
O2—Cu1—N4—C16	−59.5 (6)	C2—C1—C7—O1	−168.3 (4)
O3—Cu1—N4—C16	−166.6 (3)	C6—C1—C7—O2	−170.8 (4)
N3—Cu1—N4—C16	1.0 (3)	C2—C1—C7—O2	11.3 (7)
N5—Cu1—N4—C16	98.0 (3)	C17—N3—C8—C9	0.6 (7)
O2—Cu1—N5—C18	−138.0 (3)	Cu1—N3—C8—C9	178.4 (4)
O3—Cu1—N5—C18	−42.9 (3)	N3—C8—C9—C10	−1.4 (8)
N4—Cu1—N5—C18	48.4 (3)	C8—C9—C10—C11	0.5 (8)
N3—Cu1—N5—C18	129.5 (3)	C9—C10—C11—C17	1.0 (8)
O2—Cu1—N5—C22	51.4 (3)	C16—C12—C13—C14	0.7 (8)
O3—Cu1—N5—C22	146.5 (3)	C12—C13—C14—C15	−0.4 (8)
N4—Cu1—N5—C22	−122.3 (3)	C16—N4—C15—C14	−0.2 (7)
N3—Cu1—N5—C22	−41.1 (3)	Cu1—N4—C15—C14	180.0 (4)
O3—Cu1—O2—C7	−11.4 (4)	C13—C14—C15—N4	0.2 (8)

N4—Cu1—O2—C7	−118.0 (5)	C15—N4—C16—C12	0.4 (6)
N3—Cu1—O2—C7	−177.1 (4)	Cu1—N4—C16—C12	−179.7 (3)
N5—Cu1—O2—C7	84.6 (4)	C15—N4—C16—C17	−179.6 (4)
O2—Cu1—O3—C2	21.7 (4)	Cu1—N4—C16—C17	0.3 (5)
N4—Cu1—O3—C2	−174.2 (4)	C13—C12—C16—N4	−0.6 (7)
N3—Cu1—O3—C2	132.1 (5)	C13—C12—C16—C17	179.3 (4)
N5—Cu1—O3—C2	−77.8 (4)	C8—N3—C17—C11	1.0 (6)
Cu1—O3—C2—C3	164.5 (3)	Cu1—N3—C17—C11	−177.0 (3)
Cu1—O3—C2—C1	−18.7 (6)	C8—N3—C17—C16	−179.1 (4)
C6—C1—C2—O3	−178.2 (4)	Cu1—N3—C17—C16	2.9 (5)
C7—C1—C2—O3	−0.4 (7)	C10—C11—C17—N3	−1.8 (7)
C6—C1—C2—C3	−1.3 (6)	C10—C11—C17—C16	178.3 (4)
C7—C1—C2—C3	176.5 (4)	N4—C16—C17—N3	−2.1 (5)
O3—C2—C3—C4	177.8 (4)	C12—C16—C17—N3	177.9 (4)
C1—C2—C3—C4	0.7 (6)	N4—C16—C17—C11	177.7 (4)
O3—C2—C3—N1	−2.1 (7)	C12—C16—C17—C11	−2.2 (7)
C1—C2—C3—N1	−179.2 (4)	C22—N5—C18—C19	2.3 (7)
O5—N1—C3—C4	−22.6 (7)	Cu1—N5—C18—C19	−168.7 (4)
O4—N1—C3—C4	156.2 (5)	N5—C18—C19—C20	−0.4 (8)
O5—N1—C3—C2	157.3 (5)	C18—C19—C20—C21	−1.4 (8)
O4—N1—C3—C2	−23.8 (7)	C19—C20—C21—C22	1.0 (7)
C2—C3—C4—C5	0.0 (7)	C18—N5—C22—C21	−2.7 (7)
N1—C3—C4—C5	180.0 (4)	Cu1—N5—C22—C21	168.4 (4)
C3—C4—C5—C6	−0.3 (7)	C20—C21—C22—N5	1.0 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···O1^{i}	0.93	2.31	3.226 (6)	169
C22—H22A···O1^{ii}	0.93	2.47	3.174 (6)	133
C9—H9A···O6^{iii}	0.93	2.68	3.306 (6)	125
C19—H19A···O5^{iv}	0.93	2.64	3.283 (6)	126

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

Fig. 1

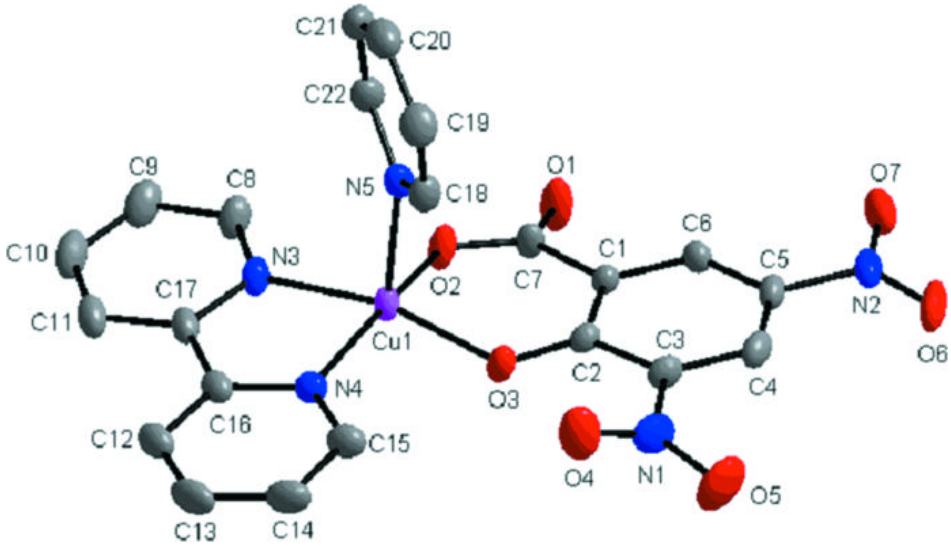
C21
C20
C22
C19
C9
C8
N5
C18
O1
O7
C10
N3
C17
O2
C7
C1
C6
C5
N2
O6
C11
Cu1
C3
C2
C4
N4
O3
C16
C12
C15
O4
N1
O5
C13
C14

Fig. 2