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(2,2′-Bipyridine-κ^2N,N')(1-formyl-2-naphtholato-κ^2O,O')(nitrato-κO)-copper(II)

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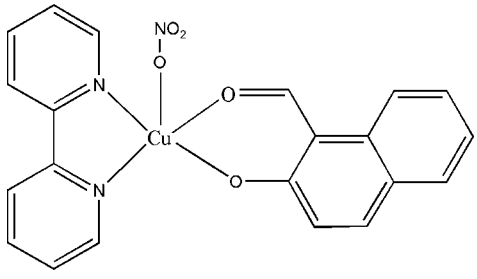
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 12.0.

In the title mononuclear complex, $[Cu(C_{11}H_7O_2)(NO_3)(C_{10}H_8N_2)]$, the Cu^{II} atom is five-coordinated in a distorted square-pyramidal environment by two N atoms of 2,2′-bipyridine, two O atoms of 1-formyl-2-naphtholate and a nitrate O atom. Molecules are stacked by π–π interactions [the dihedral angle, interplanar average distance and ring-centroid separation involved in stacking are 0.000 (1), 3.3504 (2) and 4.0800 (7) Å for stronger interactions, and 2.505 (1), 3.5373 (2) and 4.2048 (9) Å for weaker interactions] into a one-dimensional structure.

Related literature

For related literature, see: Elmali & Elerman (2002); Maniukiewicz & Bukowska-Strzyzewska (1992); Xiu-Jian et al. (2005); Yu *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{11}H_7O_2)(NO_3)(C_{10}H_8N_2)]$
M_r = 452.90
Monoclinic, $P2_1/c$
a = 12.428 (3) Å
b = 9.167 (2) Å
c = 17.245 (6) Å
β = 108.85 (1)°
V = 1859.3 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 296 (2) K
0.56 × 0.48 × 0.36 mm

Data collection

Siemens P4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.767, T_{max} = 0.985
(expected range = 0.503–0.645)
3797 measured reflections
3261 independent reflections
2552 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections
every 97 reflections
intensity decay: 1.4%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.05
3261 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.9082 (18)	Cu—N2	1.995 (2)
Cu—O2	1.934 (2)	Cu—O3	2.265 (3)
Cu—N1	1.994 (2)		
O1—Cu—O2	92.12 (8)	N1—Cu—N2	81.15 (9)
O1—Cu—N1	91.97 (9)	O1—Cu—O3	91.16 (9)
O1—Cu—N2	169.98 (9)	N2—Cu—O3	96.45 (10)
O2—Cu—N2	92.40 (9)		

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2125).

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supplementary materials

Acta Cryst. (2007). E**63**, m2358 [**doi:10.1107/S1600536807039669**]

(2,2'-Bipyridine-κ^2N,N')(1-formyl-2-naphtholato-κ^2O,O')(nitrato-κO)copper(II)

B.-R. Lian, J.-X. Li, Y.-M. Jiang and B.-L. Liang

Comment

In the previously published papers, the crystal structures of 2-hydroxy-1-naphthaldehyde (Maniukiewicz & Bukowska-Strzyzewska, 1992) and its three copper(II) complexes (Yu *et al.*, 2006; Xiu-Jian *et al.*, 2005; Elmali & Elerman, 2002) have been determined. In this paper, we report a new compound containing naphthaldehyde as a ligand (Fig.1). The Cu^{II} atom is five-coordinated by two N atoms of bipy and two O atoms of naph in the equatorial plane with an axial nitrate O—Cu bond to form square-pyramidal coordination geometry (Table 1). The Cu atom is shifted from from the least-squares plane N1/N2/O2/O1 by 0.2103 (3)Å towards O3. The presented structure comprises the same cation as $[Cu(C_{10}H_8N_2)(C_{11}H_7O_2)(ClO_4)]$ (Elmali & Elerman, 2002) but anions are different: nitrate and perchlorate. In the crystal structure of (I), there are two kinds of π-π stacking interactions: strong one between naphthalene rings (symmetry codes: $-x+1, y-1/2, -z+1/2$; $x, -y+3/2, z+1/2$) and the weak one between naphthalene ring and pyridine ring (symmetry codes: $-x+1, y-1/2, -z+1/2$; $x, y-1/2, z+1/2$). The dihedral angle, interplanar average distance and ring-centroid separation distance are: 0.000 (1)°, 3.3504 (2) Å, 4.0800 (7)Å for the former ones and 2.505 (1)°, 3.5373 (2) Å, 4.2048 (9)Å for the latter ones, respectively. The title molecules are connected into dimers through the first kind of stacking and further linked into a one-dimensional skeleton *via* the second π-π stacking along *c* axis (Fig. 2).

Experimental

A 10 ml me thanol solution of $Cu(NO_3)_2{\cdot}3H_2O$ (0.242 g,1 mmol) was dropped into 10 ml me thanol solution of 2, 2'-bipyridine(0.156 g,1 mmol) and 2-hydroxy-1-naphthaldehyde (0.16 g,1 mmol) to be stirred for 5 h at 323 K. By an evaporation of the filtrate for about 10 days green block-shaped crystals were obtained. Analysis, found (%): C, 55.60; H, 3.35; N, 9.21. $C_{21}H_{15}CuN_3O_5$ required (%):*C*, 55.64; H, 3.31; N, 9.27.

Refinement

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

Figures

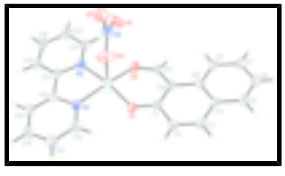

Fig. 1. The molecular structure of (I) with the atom-numbering scheme and displacement parameters scaled at the 30% probability.

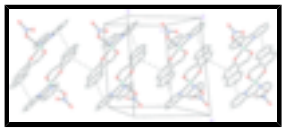

Fig. 2. Packing of (I) showing the one-dimensional structure in the *ab* plane, linked π-π stacking (dashed lines). H atoms have been omitted.

(2,2'-Bipyridine-κ^2*N*,*N*')(1-formyl-2-naphtholato-κ^2*O*,*O*')(nitrato-\ κ*O*)copper(II)

Crystal data

$[Cu(C_{11}H_7O_2)(NO_3)(C_{10}H_8N_2)]$	F_{000} = 924
M_r = 452.90	D_x = 1.618 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 38 reflections
a = 12.428 (3) Å	θ = 4.6–15.2º
b = 9.167 (2) Å	μ = 1.22 mm^{-1}
c = 17.245 (6) Å	T = 296 (2) K
β = 108.85 (1)º	Block, green
V = 1859.3 (9) Å^3	0.56 × 0.48 × 0.36 mm
Z = 4	

Data collection

Siemens P4 diffractometer	R_{int} = 0.017
Radiation source: normal-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 1.7º
T = 296(2) K	h = 0→14
ω scans	k = 0→10
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	l = −20→19
T_{min} = 0.767, T_{max} = 0.985	3 standard reflections
3797 measured reflections	every 97 reflections
3261 independent reflections	intensity decay: 1.4%
2552 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.0639P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.093	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
3261 reflections	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
272 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00014 (4)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu	0.69710 (3)	0.56548 (4)	0.01255 (2)	0.04165 (14)
O1	0.57130 (15)	0.6902 (2)	−0.03875 (11)	0.0465 (5)
O2	0.64002 (17)	0.5217 (2)	0.10181 (12)	0.0488 (5)
O3	0.8122 (2)	0.7602 (3)	0.05872 (16)	0.0885 (9)
O4	0.8697 (3)	0.6778 (3)	0.18001 (17)	0.1045 (10)
O5	0.9546 (2)	0.8586 (3)	0.14903 (16)	0.0751 (7)
N1	0.73773 (19)	0.5505 (3)	−0.08999 (14)	0.0424 (5)
N2	0.81823 (18)	0.4139 (2)	0.04854 (14)	0.0412 (5)
N3	0.8786 (2)	0.7689 (3)	0.12895 (18)	0.0549 (7)
C1	0.5021 (2)	0.7470 (3)	−0.00535 (17)	0.0408 (6)
C2	0.4219 (2)	0.8518 (3)	−0.05254 (18)	0.0473 (7)
H2	0.4195	0.8722	−0.1059	0.057*
C3	0.3493 (2)	0.9216 (3)	−0.02088 (19)	0.0488 (7)
H3	0.2982	0.9886	−0.0534	0.059*
C4	0.3487 (2)	0.8958 (3)	0.06057 (18)	0.0448 (7)
C5	0.2758 (3)	0.9761 (4)	0.0928 (2)	0.0590 (9)
H5	0.2281	1.0469	0.0609	0.071*
C6	0.2749 (3)	0.9502 (4)	0.1705 (2)	0.0664 (10)
H6	0.2272	1.0038	0.1915	0.080*
C7	0.3455 (3)	0.8437 (4)	0.2182 (2)	0.0573 (8)
H7	0.3438	0.8252	0.2708	0.069*
C8	0.4175 (2)	0.7658 (3)	0.18808 (18)	0.0492 (7)
H8	0.4647	0.6959	0.2212	0.059*
C9	0.4220 (2)	0.7884 (3)	0.10894 (17)	0.0413 (6)
C10	0.4987 (2)	0.7101 (3)	0.07414 (17)	0.0390 (6)
C11	0.5631 (2)	0.5932 (3)	0.11747 (18)	0.0445 (7)
H11	0.5467	0.5645	0.1642	0.053*
C12	0.6931 (3)	0.6285 (4)	−0.15859 (19)	0.0550 (8)
H12	0.6364	0.6959	−0.1606	0.066*
C13	0.7278 (3)	0.6129 (4)	−0.2256 (2)	0.0678 (10)
H13	0.6947	0.6684	−0.2724	0.081*
C14	0.8112 (3)	0.5152 (4)	−0.2232 (2)	0.0660 (10)
H14	0.8362	0.5042	−0.2682	0.079*

C15	0.8582 (3)	0.4327 (3)	−0.1540 (2)	0.0563 (8)
H15	0.9147	0.3647	−0.1518	0.068*
C16	0.8204 (2)	0.4523 (3)	−0.08780 (17)	0.0401 (6)
C17	0.8641 (2)	0.3727 (3)	−0.00911 (17)	0.0418 (6)
C18	0.9466 (2)	0.2650 (3)	0.0066 (2)	0.0554 (8)
H18	0.9769	0.2364	−0.0338	0.066*
C19	0.9828 (3)	0.2011 (4)	0.0830 (2)	0.0625 (9)
H19	1.0378	0.1282	0.0945	0.075*
C20	0.9380 (3)	0.2448 (4)	0.1418 (2)	0.0585 (8)
H20	0.9626	0.2031	0.1937	0.070*
C21	0.8559 (2)	0.3514 (3)	0.12283 (18)	0.0506 (7)
H21	0.8253	0.3814	0.1629	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0377 (2)	0.0452 (2)	0.0434 (2)	0.00772 (16)	0.01494 (15)	0.00289 (17)
O1	0.0394 (10)	0.0579 (12)	0.0442 (11)	0.0120 (9)	0.0163 (9)	0.0046 (10)
O2	0.0461 (11)	0.0510 (12)	0.0537 (12)	0.0101 (10)	0.0222 (10)	0.0094 (10)
O3	0.0918 (19)	0.0642 (16)	0.0767 (18)	−0.0083 (15)	−0.0184 (15)	0.0074 (14)
O4	0.133 (3)	0.104 (2)	0.0666 (18)	−0.047 (2)	0.0194 (18)	−0.0145 (17)
O5	0.0671 (15)	0.0790 (17)	0.0836 (17)	−0.0268 (14)	0.0306 (14)	−0.0271 (15)
N1	0.0400 (12)	0.0448 (13)	0.0423 (13)	0.0051 (11)	0.0131 (11)	0.0022 (11)
N2	0.0367 (12)	0.0435 (14)	0.0430 (13)	0.0038 (10)	0.0122 (10)	0.0043 (11)
N3	0.0523 (16)	0.0560 (17)	0.0592 (18)	0.0004 (14)	0.0217 (14)	−0.0173 (15)
C1	0.0320 (13)	0.0392 (14)	0.0479 (16)	−0.0014 (12)	0.0084 (12)	−0.0052 (13)
C2	0.0453 (16)	0.0486 (17)	0.0450 (17)	0.0040 (14)	0.0104 (14)	−0.0001 (14)
C3	0.0379 (15)	0.0451 (17)	0.0575 (19)	0.0083 (13)	0.0072 (14)	0.0026 (15)
C4	0.0382 (15)	0.0439 (16)	0.0508 (18)	0.0013 (12)	0.0122 (13)	−0.0083 (13)
C5	0.0515 (19)	0.058 (2)	0.067 (2)	0.0163 (15)	0.0185 (17)	−0.0033 (17)
C6	0.061 (2)	0.070 (2)	0.078 (2)	0.0111 (18)	0.0358 (19)	−0.013 (2)
C7	0.0594 (19)	0.064 (2)	0.0532 (19)	−0.0018 (17)	0.0253 (16)	−0.0111 (17)
C8	0.0470 (17)	0.0502 (18)	0.0515 (18)	0.0001 (14)	0.0173 (15)	−0.0072 (15)
C9	0.0349 (14)	0.0403 (15)	0.0474 (16)	−0.0061 (12)	0.0114 (12)	−0.0090 (13)
C10	0.0331 (13)	0.0406 (15)	0.0434 (15)	−0.0020 (12)	0.0127 (12)	−0.0040 (12)
C11	0.0423 (16)	0.0475 (17)	0.0467 (17)	0.0011 (13)	0.0185 (13)	0.0009 (13)
C12	0.0528 (18)	0.0598 (19)	0.0525 (19)	0.0175 (16)	0.0172 (15)	0.0110 (16)
C13	0.073 (2)	0.081 (2)	0.055 (2)	0.024 (2)	0.0279 (18)	0.0241 (18)
C14	0.071 (2)	0.080 (2)	0.059 (2)	0.015 (2)	0.0382 (19)	0.0156 (19)
C15	0.0525 (18)	0.062 (2)	0.062 (2)	0.0147 (16)	0.0302 (16)	0.0096 (17)
C16	0.0323 (13)	0.0416 (15)	0.0449 (16)	0.0011 (12)	0.0103 (12)	0.0019 (13)
C17	0.0328 (14)	0.0429 (15)	0.0497 (17)	−0.0019 (12)	0.0132 (13)	0.0026 (13)
C18	0.0474 (17)	0.0566 (19)	0.067 (2)	0.0157 (15)	0.0246 (16)	0.0078 (17)
C19	0.0501 (19)	0.063 (2)	0.074 (2)	0.0231 (16)	0.0193 (17)	0.0189 (18)
C20	0.0518 (18)	0.063 (2)	0.0549 (19)	0.0085 (17)	0.0093 (16)	0.0190 (17)
C21	0.0472 (17)	0.0568 (19)	0.0474 (18)	0.0032 (15)	0.0149 (14)	0.0057 (15)

Geometric parameters (Å, °)

Cu—O1	1.9082 (18)	C6—H6	0.9300
Cu—O2	1.934 (2)	C7—C8	1.372 (4)
Cu—N1	1.994 (2)	C7—H7	0.9300
Cu—N2	1.995 (2)	C8—C9	1.399 (4)
Cu—O3	2.265 (3)	C8—H8	0.9300
O1—C1	1.289 (3)	C9—C10	1.468 (4)
O2—C11	1.259 (3)	C10—C11	1.400 (4)
O3—N3	1.228 (3)	C11—H11	0.9300
O4—N3	1.244 (4)	C12—C13	1.365 (4)
O5—N3	1.215 (3)	C12—H12	0.9300
N1—C12	1.339 (4)	C13—C14	1.360 (4)
N1—C16	1.357 (3)	C13—H13	0.9300
N2—C21	1.342 (4)	C14—C15	1.374 (4)
N2—C17	1.350 (3)	C14—H14	0.9300
C1—C10	1.426 (4)	C15—C16	1.379 (4)
C1—C2	1.434 (4)	C15—H15	0.9300
C2—C3	1.356 (4)	C16—C17	1.481 (4)
C2—H2	0.9300	C17—C18	1.385 (4)
C3—C4	1.427 (4)	C18—C19	1.378 (4)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.414 (4)	C19—C20	1.365 (4)
C4—C9	1.415 (4)	C19—H19	0.9300
C5—C6	1.363 (5)	C20—C21	1.375 (4)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.390 (5)	C21—H21	0.9300
O1—Cu—O2	92.12 (8)	C7—C8—C9	121.9 (3)
O1—Cu—N1	91.97 (9)	C7—C8—H8	119.1
O2—Cu—N1	162.68 (9)	C9—C8—H8	119.1
O1—Cu—N2	169.98 (9)	C8—C9—C4	117.2 (3)
O2—Cu—N2	92.40 (9)	C8—C9—C10	124.2 (3)
N1—Cu—N2	81.15 (9)	C4—C9—C10	118.6 (3)
O1—Cu—O3	91.16 (9)	C11—C10—C1	120.3 (2)
O2—Cu—O3	103.65 (10)	C11—C10—C9	119.4 (3)
N1—Cu—O3	93.08 (10)	C1—C10—C9	120.2 (2)
N2—Cu—O3	96.45 (10)	O2—C11—C10	128.8 (3)
C1—O1—Cu	126.84 (18)	O2—C11—H11	115.6
C11—O2—Cu	124.22 (19)	C10—C11—H11	115.6
N3—O3—Cu	123.0 (2)	N1—C12—C13	122.6 (3)
C12—N1—C16	118.2 (2)	N1—C12—H12	118.7
C12—N1—Cu	126.5 (2)	C13—C12—H12	118.7
C16—N1—Cu	115.28 (18)	C14—C13—C12	119.3 (3)
C21—N2—C17	119.0 (2)	C14—C13—H13	120.4
C21—N2—Cu	126.1 (2)	C12—C13—H13	120.4
C17—N2—Cu	114.94 (18)	C13—C14—C15	119.6 (3)
O5—N3—O3	122.5 (3)	C13—C14—H14	120.2
O5—N3—O4	119.4 (3)	C15—C14—H14	120.2

O3—N3—O4	118.0 (3)	C14—C15—C16	119.0 (3)
O1—C1—C10	124.4 (2)	C14—C15—H15	120.5
O1—C1—C2	117.3 (3)	C16—C15—H15	120.5
C10—C1—C2	118.2 (2)	N1—C16—C15	121.4 (3)
C3—C2—C1	121.3 (3)	N1—C16—C17	113.8 (2)
C3—C2—H2	119.4	C15—C16—C17	124.9 (3)
C1—C2—H2	119.4	N2—C17—C18	121.2 (3)
C2—C3—C4	122.3 (3)	N2—C17—C16	114.8 (2)
C2—C3—H3	118.9	C18—C17—C16	124.0 (3)
C4—C3—H3	118.9	C19—C18—C17	118.8 (3)
C5—C4—C9	120.2 (3)	C19—C18—H18	120.6
C5—C4—C3	120.6 (3)	C17—C18—H18	120.6
C9—C4—C3	119.2 (3)	C20—C19—C18	120.0 (3)
C6—C5—C4	120.4 (3)	C20—C19—H19	120.0
C6—C5—H5	119.8	C18—C19—H19	120.0
C4—C5—H5	119.8	C19—C20—C21	118.8 (3)
C5—C6—C7	120.0 (3)	C19—C20—H20	120.6
C5—C6—H6	120.0	C21—C20—H20	120.6
C7—C6—H6	120.0	N2—C21—C20	122.2 (3)
C8—C7—C6	120.4 (3)	N2—C21—H21	118.9
C8—C7—H7	119.8	C20—C21—H21	118.9
C6—C7—H7	119.8		
O2—Cu—O1—C1	17.3 (2)	C7—C8—C9—C10	178.9 (3)
N1—Cu—O1—C1	−179.5 (2)	C5—C4—C9—C8	0.6 (4)
N2—Cu—O1—C1	134.1 (4)	C3—C4—C9—C8	−179.3 (3)
O3—Cu—O1—C1	−86.4 (2)	C5—C4—C9—C10	−178.3 (3)
O1—Cu—O2—C11	−14.7 (2)	C3—C4—C9—C10	1.7 (4)
N1—Cu—O2—C11	−118.3 (3)	O1—C1—C10—C11	−8.3 (4)
N2—Cu—O2—C11	174.2 (2)	C2—C1—C10—C11	170.3 (2)
O3—Cu—O2—C11	77.0 (2)	O1—C1—C10—C9	175.7 (2)
O1—Cu—O3—N3	135.3 (3)	C2—C1—C10—C9	−5.7 (4)
O2—Cu—O3—N3	42.8 (3)	C8—C9—C10—C11	7.8 (4)
N1—Cu—O3—N3	−132.7 (3)	C4—C9—C10—C11	−173.3 (2)
N2—Cu—O3—N3	−51.3 (3)	C8—C9—C10—C1	−176.1 (3)
O1—Cu—N1—C12	9.0 (3)	C4—C9—C10—C1	2.7 (4)
O2—Cu—N1—C12	112.6 (3)	Cu—O2—C11—C10	3.8 (4)
N2—Cu—N1—C12	−178.3 (3)	C1—C10—C11—O2	11.0 (4)
O3—Cu—N1—C12	−82.3 (3)	C9—C10—C11—O2	−173.0 (3)
O1—Cu—N1—C16	−172.13 (19)	C16—N1—C12—C13	−0.1 (5)
O2—Cu—N1—C16	−68.5 (4)	Cu—N1—C12—C13	178.7 (3)
N2—Cu—N1—C16	0.55 (19)	N1—C12—C13—C14	−0.3 (6)
O3—Cu—N1—C16	96.6 (2)	C12—C13—C14—C15	0.7 (6)
O1—Cu—N2—C21	−134.5 (4)	C13—C14—C15—C16	−0.7 (5)
O2—Cu—N2—C21	−17.7 (2)	C12—N1—C16—C15	0.1 (4)
N1—Cu—N2—C21	178.5 (2)	Cu—N1—C16—C15	−178.8 (2)
O3—Cu—N2—C21	86.3 (2)	C12—N1—C16—C17	179.7 (3)
O1—Cu—N2—C17	45.2 (6)	Cu—N1—C16—C17	0.7 (3)
O2—Cu—N2—C17	161.98 (19)	C14—C15—C16—N1	0.3 (5)
N1—Cu—N2—C17	−1.86 (18)	C14—C15—C16—C17	−179.2 (3)

O3—Cu—N2—C17	−94.0 (2)	C21—N2—C17—C18	1.8 (4)
Cu—O3—N3—O5	165.6 (2)	Cu—N2—C17—C18	−177.9 (2)
Cu—O3—N3—O4	−11.3 (4)	C21—N2—C17—C16	−177.5 (2)
Cu—O1—C1—C10	−8.8 (4)	Cu—N2—C17—C16	2.8 (3)
Cu—O1—C1—C2	172.60 (18)	N1—C16—C17—N2	−2.3 (3)
O1—C1—C2—C3	−177.1 (3)	C15—C16—C17—N2	177.2 (3)
C10—C1—C2—C3	4.3 (4)	N1—C16—C17—C18	178.4 (3)
C1—C2—C3—C4	0.2 (4)	C15—C16—C17—C18	−2.1 (5)
C2—C3—C4—C5	176.8 (3)	N2—C17—C18—C19	−0.9 (5)
C2—C3—C4—C9	−3.3 (4)	C16—C17—C18—C19	178.3 (3)
C9—C4—C5—C6	−0.4 (5)	C17—C18—C19—C20	−0.4 (5)
C3—C4—C5—C6	179.5 (3)	C18—C19—C20—C21	0.8 (5)
C4—C5—C6—C7	−0.5 (5)	C17—N2—C21—C20	−1.3 (4)
C5—C6—C7—C8	1.1 (5)	Cu—N2—C21—C20	178.3 (2)
C6—C7—C8—C9	−0.8 (5)	C19—C20—C21—N2	0.1 (5)
C7—C8—C9—C4	0.0 (4)		

Fig. 1

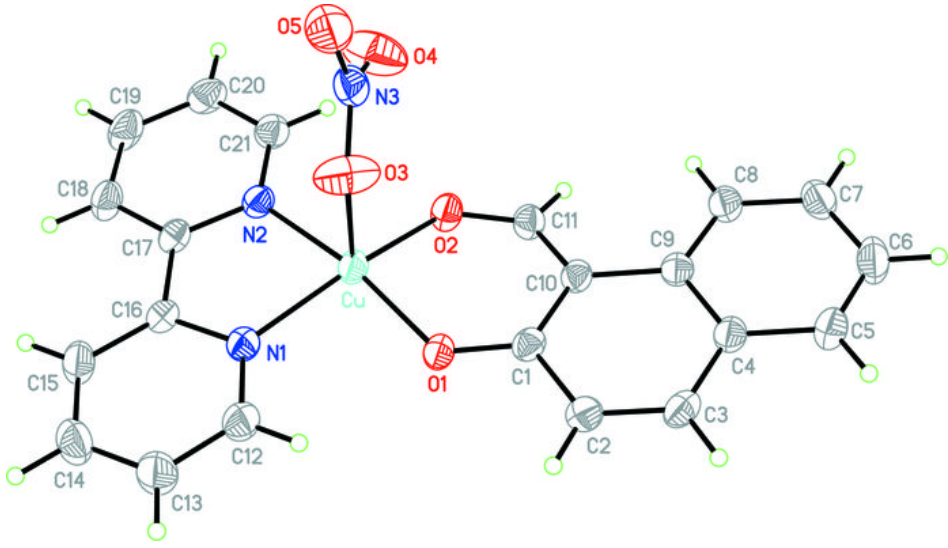
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Fig. 2