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Chlorido(di-2-pyridylamine-κ^2N,N')-(4-nitrobenzoato-κ^2O,O')copper(II)

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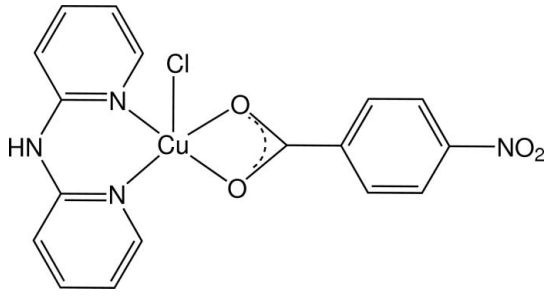
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.078; data-to-parameter ratio = 15.5.

In the title complex, $[Cu(C_7H_4NO_4)Cl(C_{10}H_9N_3)]$, the Cu atom has a distorted square-pyramidal geometry defined by one bidentate di-2-pyridylamine ligand, one bidentate 4-nitrobenzoate anion, and a Cl atom in the apical position. The Cu atom deviates from the mean plane of the basal atoms towards the Cl atom by 0.3274 (1) Å. The crystal structure is stabilized by N—H···Cl hydrogen bonds and π–π stacking interactions.

Related literature

For related literature, see: Brophy *et al.* (1999); Mao *et al.* (2004); Okabe *et al.* (2007); Wang & Okabe (2005); Yodoshi, Mototsuji & Okabe (2007); Yodoshi, Odoko & Okabe (2007); Youngme *et al.* (2004).



Experimental

Crystal data

$[Cu(C_7H_4NO_4)Cl(C_{10}H_9N_3)]$
M_r = 436.31
Triclinic, $P\overline{1}$
a = 8.87 (1) Å
b = 9.085 (8) Å
c = 11.23 (1) Å
α = 102.67 (3)°
β = 105.34 (3)°
γ = 96.72 (4)°
V = 836.6 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 123.1 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.633, T_{max} = 0.740
8197 measured reflections
3794 independent reflections
3552 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.078
S = 1.22
3794 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—Cl1	2.468 (3)	Cu1—N1	1.955 (2)
Cu1—O1	2.110 (2)	Cu1—N2	1.967 (2)
Cu1—O2	2.002 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H9···Cl1^{i}	0.86	2.33	3.163 (2)	165

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2180).

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supplementary materials

Acta Cryst. (2007). E**63**, m2162 [**doi:10.1107/S1600536807033776**]

Chlorido(di-2-pyridylamine-κ^2N,N')(4-nitrobenzoato-κ^2O,O')copper(II)

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Comment

As part of our studies of new therapeutic drugs, we have reported the structures of ternary Cu(II) complexes with the heterocyclic ligand 2,2'-bipyridylamine (bpa) and various carboxylate ligands, such as *p*-hydroxybenzenecarboxylate (*p*-HB) (Wang & Okabe, 2005), cyclobutane-1,1-dicarboxylate (Yodoshi, Mototsuji & Okabe, 2007), benzenecarboxylate (BA) (Okabe *et al.*, 2007), and glycinate (Yodoshi, Odoko & Okabe, 2007). In this study, we describe the structure of the title Cu(II) complex, (I), containing bpa and 4-nitrobenzoate (*p*-NBA) and chloride anions.

The overall structure of (I) is similar to those of the ternary Cu(II) complexes with bpa and *p*-HB (Wang & Okabe, 2005) and BA (Okabe *et al.*, 2007). The central Cu atom in (I) (Fig. 1) has a square pyramidal CuN_2O_2Cl geometry (Table 1), resulting from its coordination by two N atoms from the bpa molecule, two O atoms from the *p*-NBA anion and one Cl atom. The four basal atoms (N1, N2, O1 and O2) are neary coplanar and the Cu atom deviates from their least-squares plane towards the apical Cl atom by 0.3274 (1) Å. The O1—Cu1—O2 and N1—Cu1—N2 bite angles of 64.25 (7) and 94.71 (8) Å, respectively, are in the ranges normally observed for these complexes (Wang & Okabe, 2005; Okabe *et al.*, 2007; Yodoshi, Mototsuji & Okabe, 2007; Yodoshi, Odoko & Okabe, 2007; Youngme *et al.*, 2004). The Cu—Cl distance of 2.468 (3)Å is intermediate between the known values from 2.336 (2) to 2.733 (2) Å (Mao *et al.*, 2004; Brophy *et al.*, 1999). Such long Cu—Cl bonds are explained by the well known Jahn-Teller effect.

As shown in Fig. 2, the crystal structure is stabilized by N3—H9···Cl1^{i} hydrogen bonds [i: 2 − *x*, −*y*, 1 − *z*] as well as by three kinds of π-π stacking interactions with the distances between the centroids of the aromatic rings being 3.531 (4) Å for *Cg*1(N1/C1—C5) and *Cg*3(N2/C6—C10) at (1 − *x*, −*y*, −*z*), 3.754 (4) Å for *Cg*2(N1/C5/N3/C6/N2/Cu1) and *Cg*2 at (1 − *x*, −*y*, −*z*), and 3.549 (4) Å for *Cg*4(C12—C17) and *Cg*2 at (−*x*, −*y*, −1 − *z*).

Experimental

2,2'-Bipyridylamine (5.0 mg, 0.03 mol) dissolved in 90% (*v*/*v*) methanol–water solution (2 ml) was mixed with *p*-nitrobenzoic acid (4.9 mg, 0.03 mol), dissolved in the same solution (2 ml) for 5 min at room temperature. This was followed by the addition of $CuCl_2·2H_2O$ (5.0 mg, 0.03 mol) dissolved in H_2O (1 ml) and reacted for 15 min at room temperature. After several days, green prismatic crystals of (I) appeared from the mother liquor.

Refinement

All H atoms were placed in idealized positions and treated as riding, with C—H = 0.93 Å and N—H = 0.86, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Figures

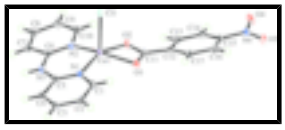

Fig. 1. A view of the molecular structure of (I) with the atomic numbering-scheme and displacement ellipsoid drawn at the 50% probability level.

Fig. 2. A view of crystal packing of (I) showing the N—H···Cl^{i} hydrogen bonds as green dashed lines [i: 2 − *x*, −*y*, 1 − *z*]. The π–π stacking interactions are shown as purple dashed lines and occur between *Cg*1(N1/C1—C5) and *Cg*3*(N2/C6—C10) [*: 1 − *x*, −*y*, −*z*], *Cg*2(N1/C5/N3C6/N2/Cu1) and *Cg*2*, and *Cg*4(C12—C17) and *Cg*2** [**: −*x*, −*y*, −1 − *z*].

Chlorido(di-2-pyridylamine-κ^2*N*,*N*')(4-nitrobenzoato-κ^2*O*,*O*')copper(II)

Crystal data

$[Cu(C_7H_4NO_4)Cl(C_{10}H_9N_3)]$	$Z = 2$
$M_r = 436.31$	$F_{000} = 442$
Triclinic, $P\overline{1}$	$D_x = 1.732$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.7107 Å
$a = 8.87$ (1) Å	Cell parameters from 7938 reflections
$b = 9.085$ (8) Å	θ = 3.0–27.5º
$c = 11.23$ (1) Å	μ = 1.50 mm^{-1}
α = 102.67 (3)º	$T = 123.1$ K
β = 105.34 (3)º	Block, green
γ = 96.72 (4)º	0.20 × 0.20 × 0.20 mm
$V = 836.6$ (14) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	3552 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.0 pixels mm^{-1}	$R_{int} = 0.014$
ω scans	$\theta_{max} = 27.5$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -11\rightarrow11$
$T_{min} = 0.633$, $T_{max} = 0.740$	$k = -11\rightarrow11$
8197 measured reflections	$l = -14\rightarrow13$
3794 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 1.3275P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.22$	$\Delta\rho_{max} = 0.47$ e Å^{-3}
3794 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
245 parameters	Extinction correction: none

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.73294 (3)	0.07819 (3)	0.27481 (3)	0.01278 (8)
Cl1	0.70600 (6)	0.23331 (6)	0.47546 (5)	0.0173 (1)
O1	0.6611 (2)	0.2345 (2)	0.1668 (2)	0.0175 (3)
O2	0.5053 (2)	0.0288 (2)	0.1663 (2)	0.0178 (3)
O3	−0.0260 (2)	0.4624 (2)	−0.1488 (2)	0.0236 (4)
O4	−0.1654 (2)	0.2565 (2)	−0.1366 (2)	0.0259 (4)
N1	0.9631 (2)	0.1289 (2)	0.3077 (2)	0.0131 (3)
N2	0.7358 (2)	−0.1247 (2)	0.3095 (2)	0.0139 (3)
N3	1.0167 (2)	−0.1001 (2)	0.3660 (2)	0.0145 (4)
N4	−0.0381 (2)	0.3401 (2)	−0.1195 (2)	0.0173 (4)
C1	1.0206 (3)	0.2650 (3)	0.2896 (2)	0.0161 (4)
C2	1.1788 (3)	0.3166 (3)	0.3095 (2)	0.0190 (4)
C3	1.2867 (3)	0.2236 (3)	0.3494 (2)	0.0177 (4)
C4	1.2313 (3)	0.0849 (3)	0.3668 (2)	0.0159 (4)
C5	1.0671 (3)	0.0395 (2)	0.3462 (2)	0.0129 (4)
C6	0.8680 (3)	−0.1814 (2)	0.3489 (2)	0.0134 (4)
C7	0.8602 (3)	−0.3277 (3)	0.3738 (2)	0.0165 (4)
C8	0.7149 (3)	−0.4120 (3)	0.3600 (2)	0.0186 (4)
C9	0.5780 (3)	−0.3515 (3)	0.3211 (2)	0.0198 (5)
C10	0.5934 (3)	−0.2102 (3)	0.2967 (2)	0.0177 (4)
C11	0.5245 (3)	0.1524 (3)	0.1326 (2)	0.0140 (4)
C12	0.3807 (3)	0.2005 (3)	0.0586 (2)	0.0131 (4)
C13	0.2366 (3)	0.0967 (3)	0.0131 (2)	0.0144 (4)
C14	0.0990 (3)	0.1430 (3)	−0.0461 (2)	0.0148 (4)
C15	0.1099 (3)	0.2917 (3)	−0.0591 (2)	0.0142 (4)
C16	0.2522 (3)	0.3956 (3)	−0.0182 (2)	0.0162 (4)
C17	0.3891 (3)	0.3480 (3)	0.0422 (2)	0.0157 (4)
H1	0.9487	0.3262	0.2624	0.019*
H2	1.2136	0.4109	0.2968	0.023*
H3	1.3951	0.2556	0.3640	0.021*
H4	1.3016	0.0214	0.3921	0.019*
H5	0.9527	−0.3664	0.3993	0.020*

H6	0.7077	−0.5082	0.3763	0.022*
H7	0.4783	−0.4061	0.3120	0.024*
H8	0.5017	−0.1708	0.2699	0.021*
H9	1.0932	−0.1453	0.3947	0.017*
H10	0.2329	−0.0028	0.0223	0.017*
H11	0.0016	0.0758	−0.0763	0.018*
H12	0.2561	0.4937	−0.0306	0.019*
H13	0.4865	0.4152	0.0716	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0089 (1)	0.0130 (1)	0.0164 (1)	0.00345 (9)	0.0011 (1)	0.0062 (1)
Cl1	0.0161 (3)	0.0200 (3)	0.0166 (3)	0.0094 (2)	0.0029 (2)	0.0057 (2)
O1	0.0115 (7)	0.0191 (8)	0.0210 (8)	0.0032 (6)	0.0013 (6)	0.0079 (7)
O2	0.0121 (7)	0.0184 (8)	0.0230 (8)	0.0045 (6)	0.0006 (6)	0.0101 (7)
O3	0.0251 (9)	0.0277 (9)	0.0240 (9)	0.0142 (7)	0.0067 (7)	0.0149 (8)
O4	0.0121 (8)	0.0298 (9)	0.033 (1)	0.0061 (7)	0.0015 (7)	0.0083 (8)
N1	0.0107 (8)	0.0150 (9)	0.0128 (8)	0.0037 (7)	0.0015 (7)	0.0040 (7)
N2	0.0134 (9)	0.0136 (8)	0.0139 (9)	0.0031 (7)	0.0021 (7)	0.0041 (7)
N3	0.0118 (8)	0.0158 (9)	0.0163 (9)	0.0069 (7)	0.0015 (7)	0.0062 (7)
N4	0.0161 (9)	0.023 (1)	0.0137 (9)	0.0096 (8)	0.0030 (7)	0.0046 (8)
C1	0.014 (1)	0.017 (1)	0.018 (1)	0.0049 (8)	0.0027 (8)	0.0075 (9)
C2	0.017 (1)	0.021 (1)	0.021 (1)	0.0023 (9)	0.0048 (9)	0.0101 (9)
C3	0.011 (1)	0.026 (1)	0.017 (1)	0.0030 (9)	0.0032 (8)	0.0064 (9)
C4	0.012 (1)	0.021 (1)	0.015 (1)	0.0071 (8)	0.0021 (8)	0.0046 (9)
C5	0.013 (1)	0.016 (1)	0.0095 (9)	0.0046 (8)	0.0019 (8)	0.0024 (8)
C6	0.016 (1)	0.013 (1)	0.0103 (9)	0.0042 (8)	0.0030 (8)	0.0025 (8)
C7	0.020 (1)	0.015 (1)	0.015 (1)	0.0074 (8)	0.0043 (9)	0.0046 (8)
C8	0.026 (1)	0.013 (1)	0.016 (1)	0.0039 (9)	0.0053 (9)	0.0041 (9)
C9	0.018 (1)	0.018 (1)	0.021 (1)	−0.0015 (9)	0.0037 (9)	0.0050 (9)
C10	0.015 (1)	0.019 (1)	0.019 (1)	0.0034 (8)	0.0034 (9)	0.0057 (9)
C11	0.012 (1)	0.016 (1)	0.013 (1)	0.0049 (8)	0.0030 (8)	0.0030 (8)
C12	0.011 (1)	0.017 (1)	0.0112 (9)	0.0051 (8)	0.0030 (8)	0.0047 (8)
C13	0.015 (1)	0.014 (1)	0.015 (1)	0.0039 (8)	0.0038 (8)	0.0055 (8)
C14	0.011 (1)	0.018 (1)	0.014 (1)	0.0022 (8)	0.0023 (8)	0.0040 (8)
C15	0.012 (1)	0.020 (1)	0.012 (1)	0.0083 (8)	0.0033 (8)	0.0056 (8)
C16	0.018 (1)	0.016 (1)	0.018 (1)	0.0065 (8)	0.0057 (9)	0.0084 (9)
C17	0.013 (1)	0.017 (1)	0.017 (1)	0.0022 (8)	0.0034 (8)	0.0055 (9)

Geometric parameters (Å, °)

Cu1—Cl1	2.468 (3)	C3—H3	0.9300
Cu1—O1	2.110 (2)	C4—C5	1.408 (3)
Cu1—O2	2.002 (3)	C4—H4	0.9300
Cu1—N1	1.955 (2)	C6—C7	1.415 (3)
Cu1—N2	1.967 (2)	C7—C8	1.372 (3)
O1—C11	1.260 (3)	C7—H5	0.9300
O2—C11	1.269 (3)	C8—C9	1.395 (4)

O3—N4	1.226 (3)	C8—H6	0.9300
O4—N4	1.228 (3)	C9—C10	1.370 (4)
N1—C1	1.359 (3)	C9—H7	0.9300
N1—C5	1.347 (3)	C10—H8	0.9300
N2—C6	1.342 (3)	C11—C12	1.495 (3)
N2—C10	1.358 (3)	C12—C13	1.395 (3)
N3—C5	1.379 (3)	C12—C17	1.388 (3)
N3—C6	1.378 (3)	C13—C14	1.386 (3)
N3—H9	0.8600	C13—H10	0.9301
N4—C15	1.474 (3)	C14—C15	1.385 (3)
C1—C2	1.368 (3)	C14—H11	0.9299
C1—H1	0.9299	C15—C16	1.385 (3)
C2—C3	1.400 (4)	C16—C17	1.392 (3)
C2—H2	0.9300	C16—H12	0.9299
C3—C4	1.372 (4)	C17—H13	0.9300
Cu1···N3	3.213 (2)	C5···H1	3.1569
Cu1···C1	2.838 (2)	C5···H3	3.2461
Cu1···C5	2.942 (2)	C5···H4	2.0415
Cu1···C6	2.947 (2)	C5···H9	1.8960
Cu1···C10	2.853 (2)	C5···H9^{ii}	3.5623
Cu1···C11	2.371 (2)	C5···H11^{i}	2.8517
Cu1···C13^{i}	3.370 (2)	C6···N3^{ii}	3.450 (3)
Cu1···H1	2.8330	C6···N4^{i}	3.454 (3)
Cu1···H8	2.8508	C6···C4^{ii}	3.489 (3)
Cu1···H9^{ii}	3.5040	C6···C5^{ii}	3.250 (3)
Cu1···H10^{i}	3.3583	C6···C8	2.405 (3)
Cl1···O1	3.385 (2)	C6···C9	2.744 (3)
Cl1···O2	3.435 (2)	C6···C10	2.317 (3)
Cl1···N1	3.412 (2)	C6···C14^{i}	3.577 (4)
Cl1···N2	3.454 (2)	C6···C15^{i}	3.254 (3)
Cl1···N3^{ii}	3.163 (2)	C6···H5	2.0484
Cl1···C3^{iii}	3.594 (2)	C6···H6	3.2513
Cl1···H2^{iv}	3.5169	C6···H8	3.1516
Cl1···H3^{iii}	2.7616	C6···H9	1.8947
Cl1···H4^{ii}	3.0162	C6···H9^{ii}	3.5643
Cl1···H5^{ii}	2.9570	C7···O3^{i}	3.328 (3)
Cl1···H6^{v}	2.8114	C7···N1^{ii}	3.471 (3)
Cl1···H7^{vi}	3.4427	C7···N4^{i}	3.597 (4)
Cl1···H9^{ii}	2.3252	C7···C1^{ii}	3.539 (3)
O1···O2	2.188 (2)	C7···C4^{ii}	3.586 (3)
O1···N1	3.102 (2)	C7···C5^{ii}	3.476 (3)
O1···C1	3.073 (3)	C7···C9	2.387 (3)
O1···C8^{v}	3.360 (3)	C7···C10	2.721 (3)
O1···C12	2.411 (2)	C7···H1^{xii}	3.3823

O1···C13^{i}	3.592 (3)	C7···H6	2.0098
O1···C17	2.876 (3)	C7···H7	3.2304
O1···H1	2.4514	C7···H9	2.4167
O1···H6^{v}	2.8321	C8···O1^{xii}	3.360 (3)
O1···H10^{i}	3.0638	C8···C2^{ii}	3.458 (3)
O1···H12^{vii}	3.2862	C8···C3^{ii}	3.341 (3)
O1···H13	2.5930	C8···C10	2.378 (4)
O2···N2	2.936 (3)	C8···H1^{xii}	3.5177
O2···C3^{iii}	3.526 (3)	C8···H3^{ii}	3.5456
O2···C10	2.942 (3)	C8···H5	2.0094
O2···C11^{i}	3.325 (3)	C8···H7	2.0336
O2···C12	2.375 (3)	C8···H8	3.2136
O2···C12^{i}	3.358 (3)	C8···H13^{xii}	3.2572
O2···C13	2.768 (3)	C9···C3^{ii}	3.452 (3)
O2···C13^{i}	3.555 (3)	C9···C17^{xii}	3.532 (3)
O2···H3^{iii}	3.1214	C9···H2^{xiii}	3.5802
O2···H4^{iii}	3.4882	C9···H3^{ii}	3.3874
O2···H8	2.3613	C9···H5	3.2319
O2···H10	2.4701	C9···H6	2.0311
O2···H10^{i}	3.5278	C9···H8	1.9878
O3···O3^{viii}	3.155 (3)	C9···H13^{xii}	2.9652
O3···O4	2.169 (3)	C10···C4^{ii}	3.547 (3)
O3···O4^{viii}	3.492 (2)	C10···H4^{ii}	3.3617
O3···N4^{viii}	3.017 (3)	C10···H6	3.2220
O3···C1^{vii}	3.221 (3)	C10···H7	2.0100
O3···C2^{vii}	3.171 (3)	C11···O2^{i}	3.325 (3)
O3···C7^{i}	3.328 (3)	C11···C11^{i}	3.486 (3)
O3···C14	3.539 (3)	C11···C13	2.482 (3)
O3···C15	2.314 (3)	C11···C17	2.505 (3)
O3···C15^{viii}	3.165 (3)	C11···H3^{iii}	3.1151
O3···C16	2.726 (3)	C11···H6^{v}	3.5229
O3···C16^{viii}	3.277 (3)	C11···H10	2.6259
O3···H1^{vii}	2.6489	C11···H10^{i}	3.3375
O3···H2^{vii}	2.5847	C11···H13	2.6580
O3···H5^{i}	3.0205	C12···O2^{i}	3.358 (3)
O3···H9^{i}	3.3943	C12···C3^{iii}	3.547 (4)
O3···H12	2.4516	C12···C14	2.402 (3)
O3···H12^{viii}	3.2237	C12···C15	2.733 (3)
O4···O3^{viii}	3.492 (2)	C12···C16	2.410 (3)
O4···N3^{i}	3.320 (3)	C12···H3^{iii}	3.3206
O4···C4^{i}	3.450 (3)	C12···H10	2.0291
O4···C5^{i}	3.519 (3)	C12···H11	3.2474

O4···C14	2.712 (3)	C12···H12	3.2553
O4···C15	2.321 (3)	C12···H13	2.0196
O4···C16	3.555 (3)	C13···Cu1^{i}	3.370 (2)
O4···C16^{viii}	3.532 (3)	C13···O1^{i}	3.592 (3)
O4···H4^{i}	3.2153	C13···O2^{i}	3.555 (3)
O4···H7^{ix}	3.5488	C13···N1^{i}	3.585 (2)
O4···H8^{ix}	2.8854	C13···C3^{iii}	3.588 (3)
O4···H9^{i}	3.1116	C13···C15	2.381 (3)
O4···H10^{ix}	2.9493	C13···C16	2.806 (3)
O4···H11	2.4230	C13···C17	2.421 (3)
O4···H12^{viii}	2.9466	C13···H11	2.0259
N1···N2	2.885 (3)	C13···H11^{ix}	2.8158
N1···N3	2.377 (3)	C13···H13	3.2570
N1···C2	2.401 (3)	C14···N1^{i}	3.268 (3)
N1···C3	2.780 (3)	C14···N3^{i}	3.385 (3)
N1···C4	2.400 (3)	C14···C5^{i}	3.260 (3)
N1···C6	3.016 (3)	C14···C6^{i}	3.577 (4)
N1···C7^{ii}	3.471 (3)	C14···C14^{ix}	3.461 (4)
N1···C13^{i}	3.585 (2)	C14···C16	2.438 (3)
N1···C14^{i}	3.268 (3)	C14···C17	2.791 (3)
N1···H1	1.9771	C14···H10	2.0211
N1···H2	3.2347	C14···H10^{ix}	3.1686
N1···H4	3.2326	C14···H11^{ix}	2.8401
N1···H5^{ii}	3.3535	C14···H12	3.2734
N1···H9	3.1038	C15···O3^{viii}	3.165 (3)
N1···H9^{ii}	3.4809	C15···N2^{i}	3.568 (3)
N1···H10^{i}	3.5119	C15···N3^{i}	3.322 (3)
N1···H11^{i}	2.9588	C15···C6^{i}	3.254 (3)
N2···N3	2.372 (3)	C15···C17	2.376 (3)
N2···C4^{ii}	3.502 (3)	C15···H9^{i}	3.5874
N2···C5	3.015 (3)	C15···H10	3.2263
N2···C7	2.404 (3)	C15···H11	2.0252
N2···C8	2.786 (3)	C15···H12	2.0295
N2···C9	2.401 (3)	C15···H13	3.2209
N2···C15^{i}	3.568 (3)	C16···O3^{viii}	3.277 (3)
N2···H4^{ii}	3.3917	C16···O4^{viii}	3.532 (3)
N2···H5	3.2359	C16···N4^{viii}	3.571 (3)
N2···H7	3.2328	C16···H11	3.2709
N2···H8	1.9776	C16···H13	2.0231
N2···H9	3.0993	C16···H13^{vii}	2.9901
N2···H9^{ii}	3.4982	C17···C9^{v}	3.532 (3)
N3···Cl1^{ii}	3.163 (2)	C17···H2^{iii}	3.5736
N3···O4^{i}	3.320 (3)	C17···H7^{v}	3.1858

N3···N3^{ii}	3.263 (3)	C17···H10	3.2582
N3···N4^{i}	3.191 (3)	C17···H12	2.0356
N3···C4	2.384 (3)	C17···H12^{vii}	3.3505
N3···C5^{ii}	3.448 (3)	C17···H13^{vii}	2.9793
N3···C6^{ii}	3.450 (3)	H1···O3^{vii}	2.6489
N3···C7	2.383 (3)	H1···C7^{v}	3.3823
N3···C10	3.596 (3)	H1···C8^{v}	3.5177
N3···C14^{i}	3.385 (3)	H2···Cl1^{iv}	3.5169
N3···C15^{i}	3.322 (3)	H2···O3^{vii}	2.5847
N3···H4	2.5498	H2···N4^{vii}	3.5583
N3···H5	2.5496	H2···C9^{x}	3.5802
N3···H9^{ii}	3.5220	H2···C17^{xi}	3.5736
N3···H11^{i}	3.2717	H3···Cl1^{xi}	2.7616
N4···O3^{viii}	3.017 (3)	H3···O2^{xi}	3.1214
N4···N3^{i}	3.191 (3)	H3···C8^{ii}	3.5456
N4···N4^{viii}	3.356 (3)	H3···C9^{ii}	3.3874
N4···C6^{i}	3.454 (3)	H3···C11^{xi}	3.1151
N4···C7^{i}	3.597 (4)	H3···C12^{xi}	3.3206
N4···C14	2.448 (3)	H4···Cl1^{ii}	3.0162
N4···C16	2.464 (3)	H4···O2^{xi}	3.4882
N4···C16^{viii}	3.571 (3)	H4···O4^{i}	3.2153
N4···H2^{vii}	3.5583	H4···N2^{ii}	3.3917
N4···H5^{i}	3.4709	H4···C10^{ii}	3.3617
N4···H9^{i}	3.0861	H5···Cl1^{ii}	2.9570
N4···H11	2.5975	H5···O3^{i}	3.0205
N4···H12	2.6282	H5···N1^{ii}	3.3535
N4···H12^{viii}	3.1857	H5···N4^{i}	3.4709
C1···O3^{vii}	3.221 (3)	H5···C1^{xii}	3.4865
C1···C3	2.375 (3)	H5···C1^{ii}	3.3473
C1···C4	2.720 (3)	H6···Cl1^{xii}	2.8114
C1···C5	2.323 (3)	H6···O1^{xii}	2.8321
C1···C7^{ii}	3.539 (3)	H6···C2^{ii}	3.3923
C1···H2	2.0107	H6···C3^{ii}	3.5455
C1···H3	3.2191	H6···C11^{xii}	3.5229
C1···H5^{v}	3.4865	H7···Cl1^{vi}	3.4427
C1···H5^{ii}	3.3473	H7···O4^{ix}	3.5488
C1···H11^{i}	3.4228	H7···C2^{xiii}	3.4306
C2···O3^{vii}	3.171 (3)	H7···C17^{xii}	3.1858
C2···C4	2.393 (4)	H8···O4^{ix}	2.8854
C2···C5	2.752 (3)	H9···Cu1^{ii}	3.5040
C2···C8^{ii}	3.458 (3)	H9···Cl1^{ii}	2.3252

C2···H1	1.9855	H9···O3^{i}	3.3943
C2···H3	2.0341	H9···O4^{i}	3.1116
C2···H4	3.2373	H9···N1^{ii}	3.4809
C2···H6^{ii}	3.3923	H9···N2^{ii}	3.4982
C2···H7^{x}	3.4306	H9···N3^{ii}	3.5220
C3···Cl1^{xi}	3.594 (2)	H9···N4^{i}	3.0861
C3···O2^{xi}	3.526 (3)	H9···C5^{ii}	3.5623
C3···C5	2.401 (3)	H9···C6^{ii}	3.5643
C3···C8^{ii}	3.341 (3)	H9···C15^{i}	3.5874
C3···C9^{ii}	3.452 (3)	H10···Cu1^{i}	3.3583
C3···C12^{xi}	3.547 (4)	H10···O1^{i}	3.0638
C3···C13^{xi}	3.588 (3)	H10···O2^{i}	3.5278
C3···H1	3.2117	H10···O4^{ix}	2.9493
C3···H2	2.0398	H10···N1^{i}	3.5119
C3···H4	2.0081	H10···C11^{i}	3.3375
C3···H6^{ii}	3.5455	H10···C14^{ix}	3.1686
C4···O4^{i}	3.450 (3)	H11···N1^{i}	2.9588
C4···N2^{ii}	3.502 (3)	H11···N3^{i}	3.2717
C4···C6^{ii}	3.489 (3)	H11···C1^{i}	3.4228
C4···C7^{ii}	3.586 (3)	H11···C4^{i}	3.2677
C4···C10^{ii}	3.547 (3)	H11···C5^{i}	2.8517
C4···H2	3.2371	H11···C13^{ix}	2.8158
C4···H3	2.0085	H11···C14^{ix}	2.8401
C4···H9	2.4215	H12···O1^{vii}	3.2862
C4···H11^{i}	3.2677	H12···O3^{viii}	3.2237
C5···O4^{i}	3.519 (3)	H12···O4^{viii}	2.9466
C5···N3^{ii}	3.448 (3)	H12···N4^{viii}	3.1857
C5···C6	2.525 (3)	H13···C8^{v}	3.2572
C5···C6^{ii}	3.250 (3)	H13···C9^{v}	2.9652
C5···C7^{ii}	3.476 (3)	H13···C16^{vii}	2.9901
C5···C14^{i}	3.260 (3)	H13···C17^{vii}	2.9793
Cl1—Cu1—O1	95.05 (5)	C5—C4—H4	120.2593
Cl1—Cu1—O2	99.92 (5)	H4—C4—C3	120.2604
Cl1—Cu1—N1	100.33 (5)	C7—C6—N2	121.4 (2)
Cl1—Cu1—N2	101.67 (6)	C7—C6—N3	117.2 (2)
O1—Cu1—O2	64.25 (7)	C8—C7—C6	119.3 (2)
O1—Cu1—N1	99.41 (8)	C8—C7—H5	120.3604
O1—Cu1—N2	155.79 (6)	H5—C7—C6	120.3492
O2—Cu1—N1	154.99 (8)	C9—C8—C7	119.2 (2)
O2—Cu1—N2	95.41 (7)	C9—C8—H6	120.4173
N1—Cu1—N2	94.71 (8)	H6—C8—C7	120.4118
C11—O1—Cu1	85.5 (1)	C10—C9—C8	118.7 (2)

C11—O2—Cu1	90.1 (1)	C10—C9—H7	120.6607
C1—N1—Cu1	116.7 (2)	H7—C9—C8	120.6708
C1—N1—C5	118.3 (2)	H8—C10—N2	118.3692
C5—N1—Cu1	125.0 (2)	H8—C10—C9	118.3655
C6—N2—Cu1	124.8 (2)	C12—C11—O1	121.8 (2)
C6—N2—C10	118.2 (2)	C12—C11—O2	118.3 (2)
C10—N2—Cu1	117.0 (2)	C13—C12—C11	118.4 (2)
C5—N3—C6	132.6 (2)	C13—C12—C17	120.9 (2)
C5—N3—H9	113.6855	C17—C12—C11	120.6 (2)
C6—N3—H9	113.6935	C14—C13—C12	119.5 (2)
C15—N4—O3	117.7 (2)	C14—C13—H10	120.2585
C15—N4—O4	118.1 (2)	H10—C13—C12	120.2528
C2—C1—N1	123.4 (2)	C15—C14—C13	118.5 (2)
C2—C1—H1	118.2880	C15—C14—H11	120.7658
H1—C1—N1	118.2784	H11—C14—C13	120.7685
C3—C2—C1	118.2 (2)	C16—C15—N4	119.0 (2)
C3—C2—H2	120.8938	C16—C15—C14	123.2 (2)
H2—C2—C1	120.8914	C17—C16—C15	117.6 (2)
C4—C3—C2	119.4 (2)	C17—C16—H12	121.1990
C4—C3—H3	120.2966	H12—C16—C15	121.1987
H3—C3—C2	120.2991	H13—C17—C12	119.8929
C5—C4—C3	119.5 (2)	H13—C17—C16	119.8888
Cl1—Cu1—O1—C11	−95.2 (1)	N1—C1—C2—C3	0.6 (4)
Cl1—Cu1—O2—C11	87.5 (1)	C1—C2—C3—C4	0.2 (3)
Cl1—Cu1—N1—C1	−79.9 (2)	C2—C3—C4—C5	−1.0 (3)
Cl1—Cu1—N2—C6	−98.4 (2)	C3—C4—C5—N1	1.0 (3)
Cu1—O1—C11—O2	−5.5 (2)	C3—C4—C5—N3	−179.4 (2)
Cu1—O2—C11—O1	5.8 (2)	N2—C6—C7—C8	−1.4 (3)
Cu1—N1—C1—C2	179.6 (2)	C6—C7—C8—C9	0.3 (3)
Cu1—N1—C5—N3	−0.0 (2)	C7—C8—C9—C10	0.7 (4)
Cu1—N1—C5—C4	179.6 (2)	C8—C9—C10—N2	−0.7 (4)
Cu1—N2—C6—N3	−1.5 (3)	O1—C11—C12—C13	173.5 (2)
Cu1—N2—C10—C9	−178.1 (2)	C11—C12—C13—C14	174.4 (2)
C6—N3—C5—N1	3.5 (4)	C11—C12—C17—C16	−175.0 (2)
C6—N3—C5—C4	−176.2 (2)	C12—C13—C14—C15	0.6 (4)
C5—N3—C6—N2	−2.7 (4)	C13—C14—C15—N4	−178.6 (2)
O3—N4—C15—C14	−169.1 (2)	N4—C15—C16—C17	178.0 (2)
O4—N4—C15—C14	11.4 (3)	C15—C16—C17—C12	0.6 (4)

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, *y*+1, *z*; (vi) −*x*+1, −*y*, −*z*+1; (vii) −*x*+1, −*y*+1, −*z*; (viii) −*x*, −*y*+1, −*z*; (ix) −*x*, −*y*, −*z*; (x) *x*+1, *y*+1, *z*; (xi) *x*+1, *y*, *z*; (xii) *x*, *y*−1, *z*; (xiii) *x*−1, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H9···Cl1^{ii}	0.86	2.33	3.163 (2)	165

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

Fig. 1

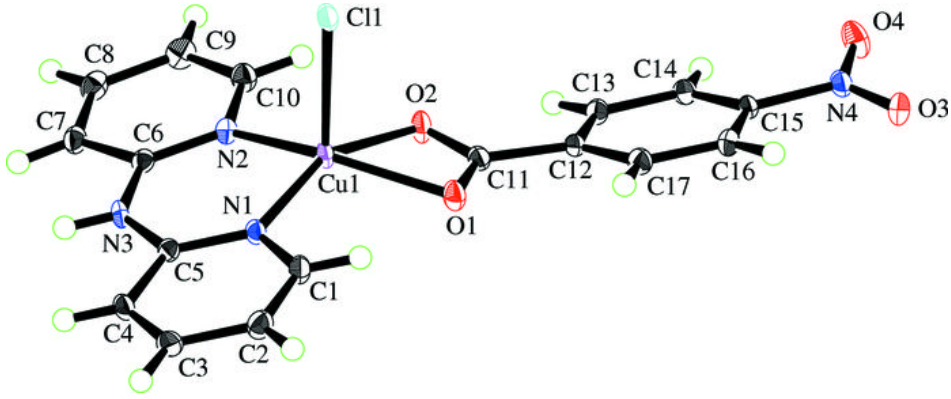
Cl1
C9
C8
C10
O2
C13
C14
O4
C7
C6
N2
Cu1
C11
C12
C15
N4
O3
C17
C16
N1
O1
N3
C5
C1
C4
C2
C3

Fig. 2