



Crystal structure and Hirshfeld surface analysis of a copper(II) complex containing 2-nitrobenzoate and tetramethylethylenediamine ligands

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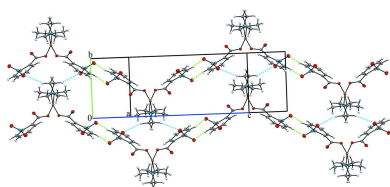
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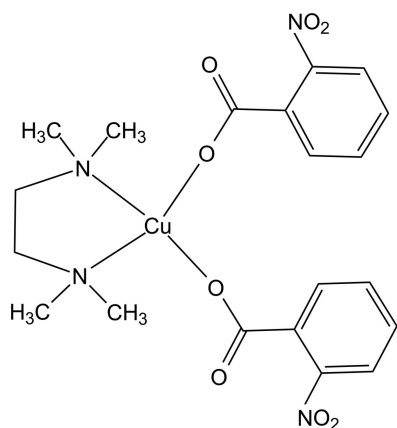
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The reaction of copper(II) sulfate pentahydrate with 2-nitrobenzoic acid and *N,N,N',N'*-tetramethylethylenediamine (TMEDA) in basic solution produces the complex bis(2-nitrobenzoato- κO)(*N,N,N',N'*-tetramethylethylenediamine- $\kappa^2 N,N'$)copper(II), $[\text{Cu}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_6\text{H}_{16}\text{N}_2)]$ or $[\text{Cu}(\text{2-nitrobenzoate})_2(\text{tmeda})]$. Each carboxylate group of the 2-nitrobenzoate ligand is coordinated by Cu^{II} atom in a monodentate fashion and two TMEDA ligand nitrogen atoms are coordinate by the metal center, giving rise to a distorted square-planar coordination environment. In the crystal, metal complexes are linked by centrosymmetric $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming ribbons *via* a $R_2^2(10)$ ring motif. These ribbons are linked by further $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, leading to two-dimensional hydrogen-bonded arrays parallel to the *bc* plane. Weak $\pi-\pi$ stacking interactions provide additional stabilization of the crystal structure. Hirshfeld surface analysis, d_{norm} and two-dimensional fingerprint plots were examined to verify the contributions of the different intermolecular contacts within the supramolecular structure. The major interactions of the complex are $\text{O}\cdots\text{H}/\text{H}\cdots\text{O}$ (44.9%), $\text{H}\cdots\text{H}$ (34%) and $\text{C}\cdots\text{H}$ (14.5%).

1. Chemical context

Copper(II) carboxylate complexes continue to be of considerable interest on account of their biological properties such as antibacterial (Melník *et al.*, 1982), antifungal (Kozlevčar *et al.*, 1999), cytotoxic and antiviral activities (Ranford *et al.*, 1993). Carboxylate ligands are versatile and can coordinate to metal centers in different modes such as monodentate, bidentate and bridging fashions. The bidentate coordination can be either symmetrical bidentate chelating, having the same C—O bond lengths, or asymmetrical bidentate chelating, having different C—O bond lengths. Carboxylate ligands have been used to generate units for developing supramolecular architectures. Copper is one of essential metals for human life. In the human body, various enzymes are copper-dependent such as Cytochrome c oxidase, superoxide dismutase, ferroxidases, monoamine oxidase, and dopamine β -monooxygenase (Brewer, 2009; Balamurugan & Schaffner, 2006). In this work, a new copper(II) complex involving 2-nitrobenzoic acid and *N,N,N',N'*-tetramethylethylenediamine was synthesized, characterized by single crystal X-ray and studied by Hirshfeld surface analysis.





2. Structural commentary

Copper(II) acetate reacts with 2-nitrobenzoic acid and *N,N,N',N'*-tetramethylethylenediamine (TMEDA) to give the mono-nuclear copper(II) complex (I). The asymmetric unit of the title compound contains one half of the metal complex, the central metal being located on the special position $4e$ ($1/2, y, 1/4$). The Cu^{II} atom has a distorted square-planar geometry with one oxygen atom each from two nitrobenzoic acid ligands and two TMEDA ligand nitrogen atoms (Figs. 1 and 2). The two nitro groups of the rings are oriented *trans* to each other, being symmetry-related to each other through a twofold axis. The structure of the complex is shown in Fig. 1. The Cu1-N1 and Cu1-O1 bond distances are 2.0269 (13) and 1.9589 (11) Å, respectively. The structural parameters of the TMEDA ligand, *i.e.* Cu-N bond lengths, are in agreement with a work reported by Gumienna-Kontecka *et al.* (2013). The C4-O1 and C4-O2 distances in the carboxyl group are 1.2772 (19) and 1.2388 (18) Å, respectively. Selected bond lengths are given in Table 1.

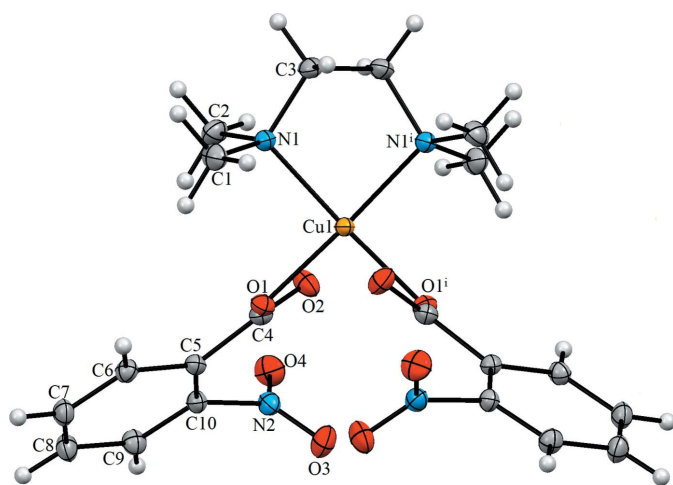


Figure 1

The molecular structure of $[\text{Cu}(\text{2-nitrobenzoate})_2(\text{tmeda})]$, with the atom labeling. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$.

Table 1
Selected bond lengths (Å).

C1-N1	1.482 (2)	Cu1-O1	1.9589 (11)
C2-N1	1.483 (2)	Cu1-N1	2.0269 (13)
C3-N1	1.490 (2)	N2-O4	1.2206 (18)
C10-N2	1.4742 (19)	N2-O3	1.2249 (19)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3-H3A}\cdots\text{O3}^{\text{i}}$	0.99	2.59	3.531 (2)	158
$\text{C9-H9}\cdots\text{O4}^{\text{ii}}$	0.95	2.42	3.291 (2)	152

Symmetry codes: (i) $-x + 1, y - 1, -z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$.

3. Supramolecular features

The crystal packing of the title complex (Fig. 2) features intermolecular hydrogen bonds ($\text{C3-H3A}\cdots\text{O3}^{\text{i}}$ and $\text{C9-H9}\cdots\text{O4}^{\text{ii}}$; symmetry codes as in Table 2). The metal complexes are self-assembled by centrosymmetric $\text{C9-H9}\cdots\text{O4}$ hydrogen bonds along the c -axis direction, forming supramolecular ribbons linked *via* $R_2^2(10)$ ring motifs. Adjacent ribbons are connected by $\text{C3-H3A}\cdots\text{O3}$ hydrogen bonds; these interactions lead to the formation of layers lying parallel to the bc plane. The three-dimensional network is stabilized by π - π stacking interactions with a centroid-to-centroid distance $\text{Cg1}\cdots\text{Cg1}^{\text{iii}}$ of 3.741 (2) Å, where Cg1 is the centroid of the C5-C10 ring [symmetry code: (iii) $-x + 1, -y + 1, -z + 1$].

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.41, update of November 2019; Groom *et al.*, 2016) for the title complex revealed four hits: *catena*- $[(\mu_2\text{-terephthalato-O,O',O'',O'''})(\mu_2\text{-terephthalato-O,O''})\text{bis}[N\text{-(2-aminoethyl)-3-amino-1-propanol}]dicopper(\text{II})]$ (FEMBEF; Mukherjee *et al.*, 2004), $\text{bis}[(\mu_2\text{-biphenyl-2,2'-dicarboxylato-O}^2,\text{O}^2')][N\text{-(pyridin-2-yl)-}N\text{pyridin-2-amine-}N^1]$ dicopper(II) tetrahydrate (GUCXOS; Kumagai *et al.*, 2009), $\text{bis}[(\mu_2\text{-biphenyl-2,2'-dicarboxylato-O}^2,\text{O}^2')][N\text{-(pyridin-2-yl)-}N\text{pyridin-2-amine-}N^1]$ dicopper(II) tetrahydrate (GUCXOS; Kumagai *et al.*, 2009), $\text{bis}[(\mu_2\text{-biphenyl-2,2'-dicarboxylato-O}^2,\text{O}^2')][N\text{-(pyridin-2-yl)-}N\text{pyridin-2-amine-}N^1]$ dicopper(II) tetrahydrate (GUCXOS; Kumagai *et al.*, 2009).

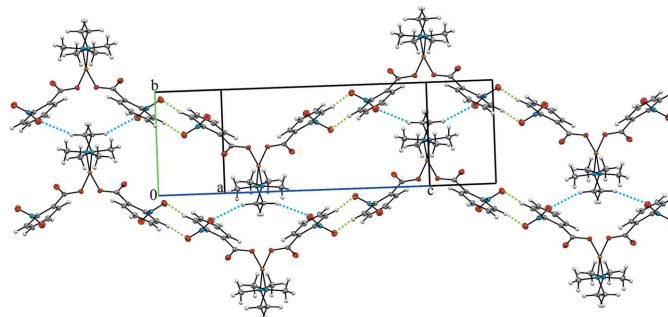


Figure 2

View of the two-dimensional hydrogen-bonded network in the structure of $[\text{Cu}(\text{2-nitrobenzoate})_2(\text{tmeda})]$ showing $\text{C9-H9}\cdots\text{O4}$ hydrogen bonds [described by an $R_2^2(10)$ ring motif] as green dashed lines and $\text{C3-H3A}\cdots\text{O3}$ hydrogen bonds as blue dashed lines.

2,2'-dicarboxylato- O^2, O^2')[N -(pyridin-2-yl- N)pyridin-2-amine- N^1]]dicopper(II) biphenyl-2,2'-dicarboxylic acid solvate monohydrate (GUCXUY; Kumagai *et al.*, 2009) and bis(2-nitrobenzoato)bis(3,5-dimethyl-1*H*-pyrazole- N^2)copper(II) (MIJFUH; Karmakar *et al.*, 2007). The Cu–N and Cu–O bond lengths range from 1.973 to 2.022 Å and 1.955 to 1.987 Å, respectively. The Cu–N and Cu–O bond lengths in the title complex [2.0269 (13) and 1.9589 (11) Å, respectively] fall within these limits.

5. Hirshfeld surface analysis

Hirshfeld surface analysis and the associated two-dimensional fingerprint plots (Spackman & Jayatilaka, 2009) are very important for explaining the intermolecular contacts in the crystal structure (Demircioğlu *et al.*, 2019; Ilmi *et al.*, 2020). We performed the Hirshfeld surface analysis with *Crystal-Explorer17* (Turner *et al.*, 2017). Fig. 3 shows the Hirshfeld surface mapped over d_{norm} (–0.2250 to 1.2935 a.u.) and the molecular electrostatic potentials (–0.2173 to 0.1248). In Fig. 3*a*, the red spots correspond to the O··H contacts. The electrostatic potential (Fig. 3*b*) shows donor (red) and acceptor (blue) regions. O··H/H··O (44.9%) contacts, seen as a pair of spikes of scattered points in the fingerprint plot, make the largest contribution to the total Hirshfeld surface in [Cu(2-nitrobenzoate)₂(tmeda)] (Fig. 4). The second most important interaction is H··H, contributing 34% to the overall crystal packing, which is shown in the 2D fingerprint of the (d_i , d_e) points related to the H atoms. Two symmetrical

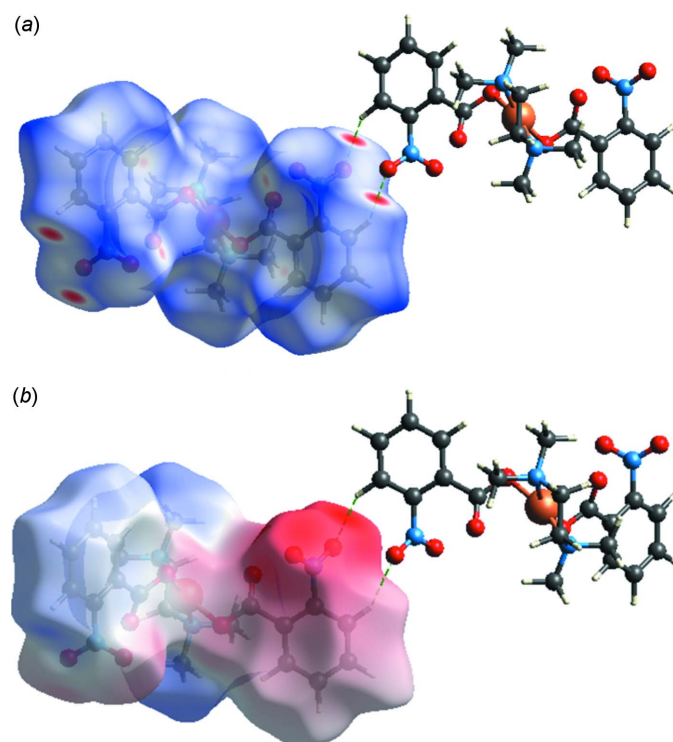


Figure 3
Hirshfeld surface of [Cu(2-nitrobenzoate)₂(tmeda)] mapped with (a) d_{norm} and (b) the molecular electrostatic potential.

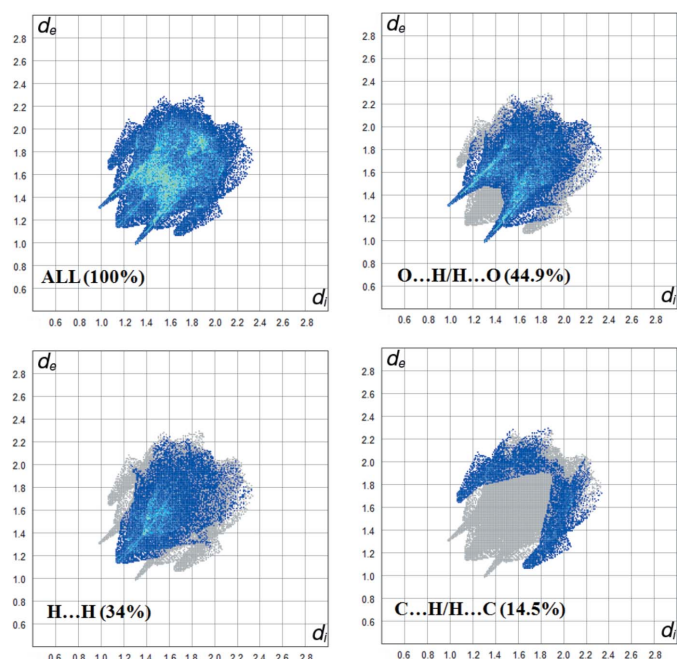


Figure 4
Two-dimensional fingerprint plots for [Cu(2-nitrobenzoate)₂(tmeda)] showing all interactions and those delineated into O··H/H··O, H··H and C··H/H··C contacts (d_i is the closest internal distance from a given point on the Hirshfeld surface and d_e is the closest external contact).

wings on the left and right sides are shown in the graph of C··H/H··C interactions (14.5%). The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of O··H, H··H and C··H interactions suggest that van der Waals interactions and hydrogen bonding play the major role in the crystal packing.

6. Synthesis and crystallization

An aqueous solution of sodium 2-nitrobenzoate (5 mmol, 0.9 g) was added to an aqueous solution of CuSO₄·5H₂O (2.5 mmol, 0.6 g) under stirring. Tetramethylethylenediamine (2.5 mmol, 0.3 g) was added and the color changed from light blue to violet. The mixture was filtered and the filtrate was allowed to stand for slow evaporation. Single crystals suitable for X-ray were obtained after several days.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically (C–H = 0.95, 0.98 and 0.99 Å) and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ otherwise.

Acknowledgements

Authors contributions are as follows. Methodology, AMQ; software, SK, ND, LY and ES; validation, SK, AMQ and ND; formal analysis, AMQ; investigation, SK, AMQ, ND and ES;

Table 3

Experimental details.

Crystal data	
Chemical formula	[Cu(C ₇ H ₄ NO ₄) ₂ (C ₆ H ₁₆ N ₂)]
<i>M</i> _r	511.97
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.7286 (3), 7.4918 (2), 22.8967 (6)
β (°)	98.395 (1)
<i>V</i> (Å ³)	2160.04 (10)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.07
Crystal size (mm)	0.22 × 0.20 × 0.12
Data collection	
Diffractometer	Bruker D8 Quest with Photon II CPADs detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2017)
<i>T</i> _{min} , <i>T</i> _{max}	0.77, 0.88
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	23494, 4737, 3573
<i>R</i> _{int}	0.056
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.808
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.092, 1.03
No. of reflections	4737
No. of parameters	152
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.55, -0.63

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT2014/5* (Sheldrick, 2015a) and *SHELXL2017/1* (Sheldrick, 2015b).

resources, AMQ and ES; writing (review and editing), SK and AMQ; visualization, SK; supervision, SK and ND; funding acquisition, LY and ES.

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supporting information

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Computing details

Data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINTE* (Bruker, 2017); data reduction: *SAINTE* (Bruker, 2017); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); software used to prepare material for publication: *APEX3* (Bruker, 2017).

Bis(2-nitrobenzoato- κ O)(*N,N,N',N'*-tetramethylethylenediamine- κ^2N,N')copper(II)

Crystal data

[Cu(C₇H₄NO₄)₂(C₆H₁₆N₂)]

$M_r = 511.97$

Monoclinic, *C2/c*

$a = 12.7286$ (3) Å

$b = 7.4918$ (2) Å

$c = 22.8967$ (6) Å

$\beta = 98.395$ (1)°

$V = 2160.04$ (10) Å³

$Z = 4$

$F(000) = 1060$

$D_x = 1.574$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6607 reflections

$\theta = 3.2\text{--}34.7^\circ$

$\mu = 1.07$ mm⁻¹

$T = 100$ K

Block, blue

0.22 × 0.20 × 0.12 mm

Data collection

Bruker D8 Quest with Photon II CPADs detector diffractometer

Radiation source: Incoatec microfocus source, Bruker D8 Quest

Multilayer Mirror monochromator

Detector resolution: 7.4074 pixels mm⁻¹

phi and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2017)

$T_{\min} = 0.77$, $T_{\max} = 0.88$

23494 measured reflections

4737 independent reflections

3573 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 35.1^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -20 \rightarrow 20$

$k = -12 \rightarrow 12$

$l = -36 \rightarrow 34$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.092$

$S = 1.03$

4737 reflections

152 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 3.2488P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.55$ e Å⁻³

$\Delta\rho_{\min} = -0.63$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.29927 (12)	0.0971 (2)	0.26549 (9)	0.0226 (3)
H1A	0.282285	0.110738	0.222582	0.034*
H1B	0.282610	0.208122	0.284815	0.034*
H1C	0.257167	-0.000768	0.278536	0.034*
C2	0.43747 (14)	0.0376 (2)	0.34649 (8)	0.0227 (3)
H2A	0.395284	-0.060381	0.359361	0.034*
H2B	0.419573	0.148951	0.365245	0.034*
H2C	0.513178	0.011891	0.357879	0.034*
C3	0.44109 (12)	-0.1106 (2)	0.25164 (8)	0.0191 (3)
H3A	0.400440	-0.116874	0.211384	0.023*
H3B	0.422415	-0.215879	0.274155	0.023*
C4	0.51601 (12)	0.4529 (2)	0.34319 (7)	0.0161 (3)
C5	0.48616 (11)	0.56860 (19)	0.39205 (7)	0.0141 (3)
C6	0.37979 (12)	0.5852 (2)	0.39976 (7)	0.0164 (3)
H6	0.326473	0.529299	0.372478	0.020*
C7	0.35056 (12)	0.6815 (2)	0.44637 (8)	0.0196 (3)
H7	0.277599	0.693902	0.450177	0.024*
C8	0.42749 (12)	0.7599 (2)	0.48755 (7)	0.0205 (3)
H8	0.407256	0.823813	0.519973	0.025*
C9	0.53414 (12)	0.7451 (2)	0.48142 (7)	0.0188 (3)
H9	0.587555	0.797819	0.509431	0.023*
C10	0.56064 (11)	0.6518 (2)	0.43364 (7)	0.0151 (3)
Cu1	0.500000	0.25244 (3)	0.250000	0.01202 (6)
N1	0.41383 (10)	0.05640 (17)	0.28142 (6)	0.0152 (2)
N2	0.67360 (10)	0.65314 (18)	0.42590 (6)	0.0176 (3)
O1	0.44317 (9)	0.43232 (14)	0.29904 (5)	0.0165 (2)
O2	0.60401 (9)	0.37907 (16)	0.34882 (6)	0.0226 (2)
O3	0.69761 (10)	0.73929 (18)	0.38435 (6)	0.0275 (3)
O4	0.73708 (9)	0.57614 (18)	0.46249 (6)	0.0268 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0144 (6)	0.0213 (7)	0.0324 (10)	-0.0007 (6)	0.0050 (6)	-0.0020 (7)
C2	0.0297 (8)	0.0196 (7)	0.0197 (8)	-0.0011 (6)	0.0063 (7)	0.0039 (6)
C3	0.0187 (6)	0.0126 (6)	0.0265 (8)	-0.0024 (5)	0.0054 (6)	-0.0010 (6)
C4	0.0175 (6)	0.0128 (6)	0.0184 (7)	-0.0012 (5)	0.0039 (5)	-0.0002 (5)
C5	0.0144 (6)	0.0124 (6)	0.0159 (7)	0.0005 (5)	0.0030 (5)	0.0005 (5)
C6	0.0140 (6)	0.0167 (6)	0.0187 (7)	-0.0013 (5)	0.0025 (5)	0.0003 (6)

C7	0.0161 (6)	0.0231 (7)	0.0211 (8)	0.0007 (6)	0.0073 (6)	0.0002 (6)
C8	0.0201 (6)	0.0241 (7)	0.0189 (7)	0.0001 (6)	0.0073 (6)	-0.0038 (7)
C9	0.0178 (6)	0.0204 (6)	0.0181 (7)	-0.0009 (6)	0.0026 (5)	-0.0021 (6)
C10	0.0131 (6)	0.0149 (6)	0.0177 (7)	0.0004 (5)	0.0036 (5)	-0.0002 (5)
Cu1	0.01247 (10)	0.01009 (10)	0.01356 (12)	0.000	0.00210 (8)	0.000
N1	0.0149 (5)	0.0127 (5)	0.0186 (6)	-0.0002 (4)	0.0040 (5)	0.0006 (5)
N2	0.0145 (5)	0.0174 (6)	0.0214 (7)	-0.0017 (5)	0.0037 (5)	-0.0035 (5)
O1	0.0189 (5)	0.0143 (5)	0.0161 (5)	0.0004 (4)	0.0021 (4)	-0.0023 (4)
O2	0.0180 (5)	0.0237 (6)	0.0262 (6)	0.0038 (4)	0.0038 (5)	-0.0065 (5)
O3	0.0213 (5)	0.0332 (7)	0.0297 (7)	-0.0039 (5)	0.0092 (5)	0.0044 (6)
O4	0.0165 (5)	0.0295 (7)	0.0329 (7)	0.0040 (5)	-0.0013 (5)	0.0026 (6)

Geometric parameters (Å, °)

C1—N1	1.482 (2)	C5—C6	1.396 (2)
C1—H1A	0.9800	C6—C7	1.383 (2)
C1—H1B	0.9800	C6—H6	0.9500
C1—H1C	0.9800	C7—C8	1.387 (2)
C2—N1	1.483 (2)	C7—H7	0.9500
C2—H2A	0.9800	C8—C9	1.389 (2)
C2—H2B	0.9800	C8—H8	0.9500
C2—H2C	0.9800	C9—C10	1.381 (2)
C3—N1	1.490 (2)	C9—H9	0.9500
C3—C3 ⁱ	1.513 (3)	C10—N2	1.4742 (19)
C3—H3A	0.9900	Cu1—O1	1.9589 (11)
C3—H3B	0.9900	Cu1—O1 ⁱ	1.9589 (11)
C4—O2	1.2388 (18)	Cu1—N1	2.0269 (13)
C4—O1	1.2772 (19)	Cu1—N1 ⁱ	2.0269 (13)
C4—C5	1.508 (2)	N2—O4	1.2206 (18)
C5—C10	1.389 (2)	N2—O3	1.2249 (19)
N1—C1—H1A	109.5	C6—C7—H7	119.9
N1—C1—H1B	109.5	C8—C7—H7	119.9
H1A—C1—H1B	109.5	C7—C8—C9	120.04 (15)
N1—C1—H1C	109.5	C7—C8—H8	120.0
H1A—C1—H1C	109.5	C9—C8—H8	120.0
H1B—C1—H1C	109.5	C10—C9—C8	118.42 (14)
N1—C2—H2A	109.5	C10—C9—H9	120.8
N1—C2—H2B	109.5	C8—C9—H9	120.8
H2A—C2—H2B	109.5	C9—C10—C5	123.28 (14)
N1—C2—H2C	109.5	C9—C10—N2	116.55 (13)
H2A—C2—H2C	109.5	C5—C10—N2	120.05 (13)
H2B—C2—H2C	109.5	O1—Cu1—O1 ⁱ	93.07 (7)
N1—C3—C3 ⁱ	108.76 (11)	O1—Cu1—N1	91.76 (5)
N1—C3—H3A	109.9	O1 ⁱ —Cu1—N1	165.06 (5)
C3 ⁱ —C3—H3A	109.9	O1—Cu1—N1 ⁱ	165.06 (5)
N1—C3—H3B	109.9	O1 ⁱ —Cu1—N1 ⁱ	91.76 (5)
C3 ⁱ —C3—H3B	109.9	N1—Cu1—N1 ⁱ	87.13 (7)

H3A—C3—H3B	108.3	C1—N1—C2	108.35 (13)
O2—C4—O1	124.71 (15)	C1—N1—C3	110.27 (12)
O2—C4—C5	120.10 (14)	C2—N1—C3	110.70 (13)
O1—C4—C5	115.09 (13)	C1—N1—Cu1	109.12 (10)
C10—C5—C6	116.79 (14)	C2—N1—Cu1	112.61 (10)
C10—C5—C4	123.09 (13)	C3—N1—Cu1	105.77 (9)
C6—C5—C4	119.95 (13)	O4—N2—O3	124.54 (14)
C7—C6—C5	121.26 (14)	O4—N2—C10	118.28 (14)
C7—C6—H6	119.4	O3—N2—C10	117.09 (13)
C5—C6—H6	119.4	C4—O1—Cu1	104.50 (9)
C6—C7—C8	120.18 (14)		
O2—C4—C5—C10	24.2 (2)	C4—C5—C10—C9	-174.19 (15)
O1—C4—C5—C10	-159.09 (14)	C6—C5—C10—N2	-174.93 (13)
O2—C4—C5—C6	-150.89 (15)	C4—C5—C10—N2	9.9 (2)
O1—C4—C5—C6	25.8 (2)	C3 ⁱ —C3—N1—C1	157.97 (16)
C10—C5—C6—C7	0.6 (2)	C3 ⁱ —C3—N1—C2	-82.14 (18)
C4—C5—C6—C7	175.98 (15)	C3 ⁱ —C3—N1—Cu1	40.11 (18)
C5—C6—C7—C8	-1.8 (2)	C9—C10—N2—O4	67.41 (19)
C6—C7—C8—C9	1.3 (3)	C5—C10—N2—O4	-116.36 (17)
C7—C8—C9—C10	0.2 (2)	C9—C10—N2—O3	-109.26 (17)
C8—C9—C10—C5	-1.5 (2)	C5—C10—N2—O3	66.97 (19)
C8—C9—C10—N2	174.64 (15)	O2—C4—O1—Cu1	4.07 (19)
C6—C5—C10—C9	1.0 (2)	C5—C4—O1—Cu1	-172.47 (10)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3A \cdots O3 ⁱⁱ	0.99	2.59	3.531 (2)	158
C9—H9 \cdots O4 ⁱⁱⁱ	0.95	2.42	3.291 (2)	152

Symmetry codes: (ii) $-x+1, y-1, -z+1/2$; (iii) $-x+3/2, -y+3/2, -z+1$.