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Crystal structure of a tetranuclear copper(II) complex with 1,10-phenanthroline and 3-nitrophthalate ligands

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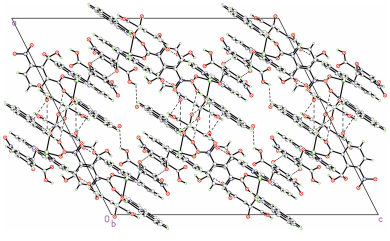
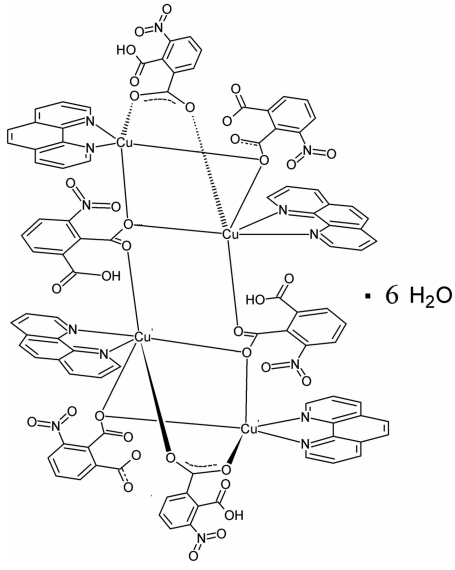
In the hydrated complex tetrakis(μ-2-carboxy-6-nitrobenzoato-κ^2O:O')bis(μ-3-nitrobenzene-1,2-dicarboxylato-κ^2O:O')tetrakis[(1,10-phenanthroline-κN:N')-copper(II)] hexahydrate, $[Cu_4(C_8H_4NO_6)_4(C_8H_3NO_6)_2(C_{12}H_8N_2)_4]\cdot 6H_2O$, the Cu^{II} centres exhibit distorted coordination geometries defined by nitrogen atoms from chelating 1,10-phenanthroline ligands and oxygen atoms from 3-nitrophthalate anions. The centrosymmetric molecular assembly is consolidated by bridging carboxylate groups, while the crystal packing is governed by hydrogen bonding and π–π stacking interactions between aromatic rings. The scattering contribution of one disordered water molecule contribution was treated using the SQUEEZE procedure.

1. Chemical context

Aromatic diimine ligands such as 1,10-phenanthroline are widely employed in coordination chemistry owing to their strong chelating ability, rigid planar geometry, and pronounced π-acceptor character (Constable, 1987). Copper(II) complexes incorporating phenanthroline frequently exhibit diverse structural motifs and supramolecular behaviour. Polycarboxylate ligands derived from 3-nitrophthalic acid represent versatile building units capable of multiple coordination modes. The presence of carboxylate and nitro functionalities enables structural diversity and promotes the formation of multinuclear assemblies (Thompson, 2002).





In the present work, we report how the combination of Cu^{II}, 1,10-phenanthroline ($C_{12}H_8N_2$) and 3-nitrophthalic acid ($C_8H_4NO_6$) in the mixed solvents of *N*,*N*-dimethylformamide, ethanol and water results in the title tetranuclear copper complex, $[Cu_4(C_8H_4NO_6)_4(C_8H_3NO_6)_2(C_{12}H_8N_2)_4]\cdot 6H_2O$ (**I**).

2. Structural commentary

The structure of (**I**) consists of a centrosymmetric, tetranuclear, copper(II) grouping in which the metal centres are interconnected by 3-nitrophthalate ligands and further ligated by chelating 1,10-phenanthroline donors. Two crystallographically independent copper atoms are present in the asymmetric unit (Fig. 1).

Atom Cu1 is five-coordinate and adopts a distorted square-pyramidal geometry. The basal plane is defined by two nitrogen atoms from one chelating phenanthroline ligand and two oxygen atoms from carboxylate groups (Table 1). The apical position is occupied by atom O4: the pronounced elongation of this axial Cu—O bond relative to the equatorial distances is consistent with the expected Jahn–Teller distortion of a $3d^9$ Cu^{II} centre.

Atom Cu2 is four-coordinate within the asymmetric unit and exhibits a distorted square-planar geometry defined by two nitrogen atoms from phenanthroline and two oxygen atoms from carboxylate groups. These Cu—O and Cu—N bond lengths fall within the typical ranges observed for Cu^{II} complexes containing carboxylate and diimine ligands.

The 3-nitrophthalate ligand acts as a μ_2-bridging linker connecting adjacent copper(II) centres. Atom O4 functions as an asymmetric carboxylate bridge between Cu1 and Cu2, coordinating axially to Cu1 [Cu1—O4 = 2.314 (3) Å] and equatorially to Cu2 [Cu2—O4 = 1.972 (3) Å]. The significant difference in bond lengths indicates stronger equatorial coordination to Cu2 and a weaker axial interaction with Cu1, consistent with Jahn–Teller distortion commonly observed for Cu^{II} centres.

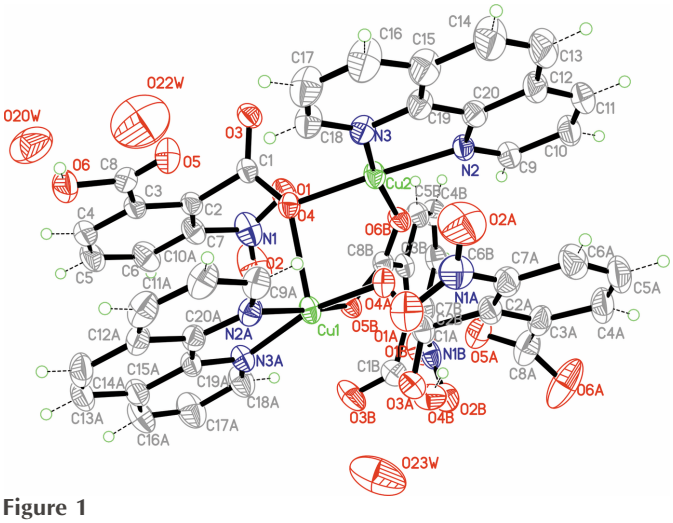


Figure 1
The molecular structure of the asymmetric unit of (**I**) with displacement ellipsoids drawn at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

Cu1—O5*B*	1.953 (3)	Cu2—O6*B*	1.944 (3)
Cu1—O4*A*	1.962 (3)	Cu2—O4	1.972 (3)
Cu1—N3*A*	1.999 (4)	Cu2—N2	2.013 (4)
Cu1—N2*A*	2.009 (4)	Cu2—N3	2.014 (4)
Cu1—O4	2.314 (3)	Cu2—O4*A*	2.484 (3)
O5*B*—Cu1—O4*A*	95.02 (12)	N3*A*—Cu1—O4	111.85 (15)
O5*B*—Cu1—N3*A*	90.89 (14)	N2*A*—Cu1—O4	85.08 (14)
O4*A*—Cu1—N3*A*	163.85 (16)	O6*B*—Cu2—O4	91.81 (12)
O5*B*—Cu1—N2*A*	169.40 (14)	O6*B*—Cu2—N2	89.88 (14)
O4*A*—Cu1—N2*A*	94.28 (15)	O4—Cu2—N2	175.61 (14)
N3*A*—Cu1—N2*A*	81.49 (16)	O6*B*—Cu2—N3	169.52 (15)
O5*B*—Cu1—O4	90.99 (12)	O4—Cu2—N3	96.28 (14)
O4*A*—Cu1—O4	83.11 (12)	N2—Cu2—N3	81.59 (16)

Additional carboxylate oxygen atoms, O5*B* and O6*B*, coordinate to Cu1 and Cu2, respectively, further consolidating the tetranuclear Cu_4 core through μ_2-carboxylate bridges (Fig. 2).

The C8*A*—O5*A* and C8*A*—O6*A* bond lengths [1.261 (7) and 1.256 (8) Å, respectively] are nearly identical, indicating delocalization within the carboxylate group and confirming its deprotonated state. Accordingly, this nitrophthalate ligand is presumed to be present in a doubly deprotonated form.

Taking into account the presence of two such dianionic ligands together with four monodeprotonated nitrophthalate ligands and four Cu^{II} centres, the overall charge of the complex is balanced.

3. Supramolecular features

In the crystal, aromatic π–π stacking interactions are observed between symmetry-related aromatic rings. The centroid–centroid separation is 3.687 (3) Å for the $Cg1\cdots Cg2^{i}$ interaction [symmetry code: (i) $1-x, 1-y, 1-z$; *Cg*1 is the centroid of the N2/C9–C12/C20 pyridyl ring of the phenanthroline ligand and *Cg*2 is the centroid of the C2–C7 benzene ring of the nitrophthalate ligand].

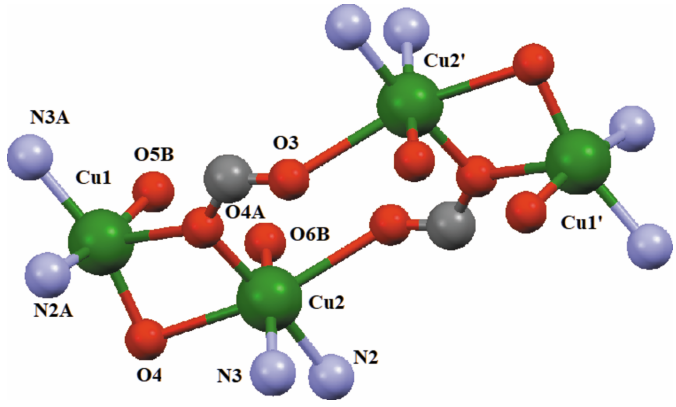


Figure 2
Simplified representation of the tetranuclear Cu_4 core in (**I**) showing the butterfly-type arrangement and the μ_2-carboxylate bridges. Primed atoms are generated by the symmetry operation $1-x, 1-y, 1-z$.

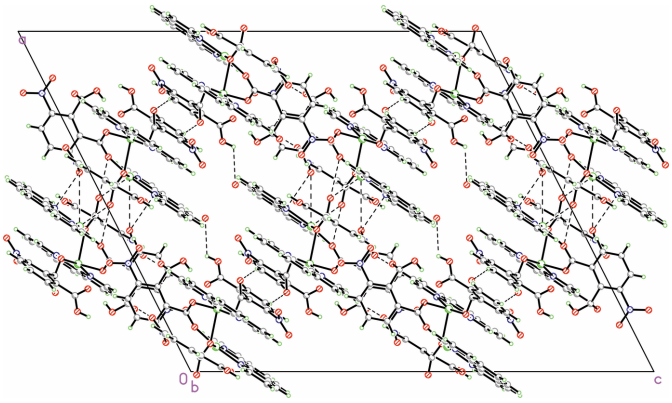


Figure 3
Crystal packing of (**I**) viewed along the [010] direction.

The interplanar separation is 3.665 Å, with a dihedral angle of 4.0 (3)°, indicating that the rings are nearly parallel. The very small slippage (ca 0.4 Å) suggests an almost face-to-face arrangement of the interacting aromatic systems (Moulton & Zaworotko, 2001).

O—H···O and C—H···O hydrogen bonds (Table 2) are also present. The packing is showin in Fig. 3.

4. Hirshfeld surface analysis

Hirshfeld surface analysis was performed using *CrystalExplorer* (Turner *et al.*, 2017; Spackman *et al.*, 2021) to quantify the intermolecular interactions in the crystal structure.

The Hirshfeld surface mapped over d_{norm} displays prominent red regions corresponding to short O···H/H···O contacts, confirming the dominant role of hydrogen bonding in consolidate the crystal packing. (Fig. 4). Two-dimensional fingerprint plots (Fig. 5) show that O···H/H···O contacts contribute 43.6%, followed by H···H interactions (25.5%). C···H/H···C contacts account for 7.5%, while O···O (4.6%), O···C/C···O (4.4%) and O···N/N···O (1.5%) interactions provide minor contributions. These results confirm that hydrogen bonding and dispersion interactions dominate the supramolecular architecture.

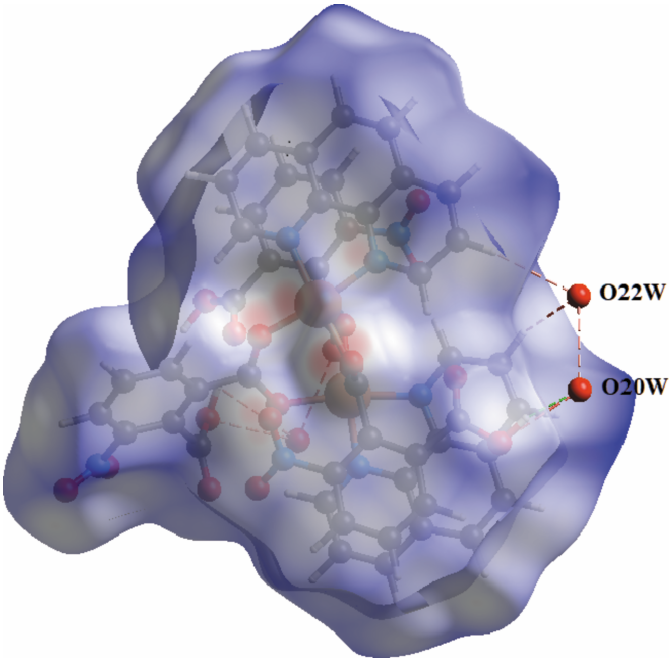


Figure 4
The Hirshfeld surface of (**I**) mapped over d_{norm} showing short intermolecular O···H/H···O contacts as red regions.

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6···O20*W*	0.82	1.84	2.649 (7)	168
C9—H9···O6*B*	0.93	2.48	2.972 (6)	113
C9*A*—H9*A*···O1*A*	0.93	2.52	3.217 (7)	132
C18—H18···O5	0.93	2.24	3.150 (7)	166
C18*A*—H18*A*···O5*B*	0.93	2.55	3.017 (6)	112
C18*A*—H18*A*···O3*B*	0.93	2.46	3.365 (7)	165
C6—H6*C*···O3*B*^{i}	0.93	2.58	3.252 (7)	129
C17*A*—H17*A*···O2^{i}	0.93	2.11	3.027 (8)	169
O4*B*—H4*B*···O5*A*	0.88 (6)	1.70 (6)	2.512 (7)	151 (6)

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

5. SQUEEZE treatment

Examination of the difference-Fourier map revealed regions of diffuse residual electron density located within solvent-accessible voids, consistent with the presence of highly disordered solvent molecules. Attempts to model this electron density using discrete atomic positions resulted in unstable refinements. Accordingly, the solvent contribution was treated using the SQUEEZE (Spek, 2015) procedure implemented in *PLATON* (Spek, 2020). The procedure identified solvent-accessible voids with volumes of approximately 10–48 Å^3, containing up to 13 electrons per void and resulted in stable refinement behaviour and chemically reasonable structural parameters. The reported molecular formula, density, *etc.* refer only to the ordered portion of the structure.

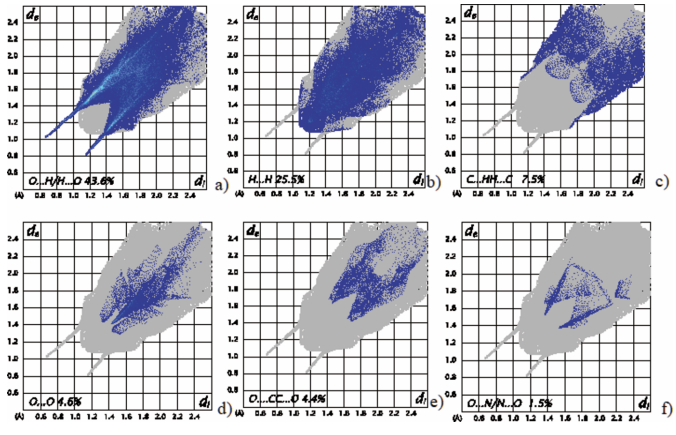


Figure 5
The two-dimensional fingerprint plots for (**I**) showing the percentage contributions of (*a*) O···H/H···O, (*b*) H···H, (*c*) C···H/H···C, (*d*) O···O, (*e*) O···C/C···O and (*f*) O···N/N···O contacts.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu_4(C_8H_4NO_6)_4(C_8H_3NO_6)_2(C_{12}H_8N_2)_4]\cdot 6H_2O$
M_r	2329.69
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	24.890 (3), 14.3705 (7), 30.179 (3)
β (°)	116.919 (12)
V (Å^3)	9624.8 (17)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.90
Crystal size (mm)	0.04 × 0.03 × 0.01
Data collection	
Diffractometer	Xcalibur, Ruby
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent Technologies, 2014)
T_{min}, T_{max}	0.916, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33685, 9915, 5785
R_{int}	0.057
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.632
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.181, 1.01
No. of reflections	9915
No. of parameters	707
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.30

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*) and *SHELXL2025/1* (Sheldrick, 2015*b*).

6. Database survey

A search of the Cambridge Structural Database (CSD Version 2025.3.1; Groom *et al.*, 2016) for structures containing both '1,10-phenanthroline' and 'Cu^{2+}' yielded 359 hits, highlighting the widespread use of phenanthroline as a chelating ligand in copper(II) coordination chemistry.

A more specific search combining the terms 'phenanthroline + $Cu2^+$ + benzenecarboxylic acid' returned ten entries (CSD refcodes ETTIE, BOVCAT, CAMZIA, CODVOJ, DOGDVB, HOPYAM, TEJXEL, XEHTEL, RADYIF and CABCIV). Among these, the structures with refcodes RADYIF (Zhu *et al.*, 2004) and CABCIV (Pinto *et al.*, 2020) represent the structurally closest known analogues to the present compound.

RADYIF features a ladder-like tetranuclear Cu_4 core sustained by μ_2- and μ_3-carboxylate bridges in combination with chelating 1,10-phenanthroline ligands. Similarly, the stepped tetranuclear core in CABCIV exhibits mixed square-planar and square-pyramidal coordination geometries around the Cu^{II} centres, consistent with the Jahn–Teller distortion typically observed for $3d^9$ metal ions.

Despite these structural similarities, the title compound is distinguished by the presence of six 3-nitrophthalate ligands per Cu_4 unit, resulting in an increased degree of μ_2-carboxylate connectivity and a more extensively bridged metal framework. In contrast to RADYIF and CABCIV, the present structure displays a higher ligand-to-metal bridging ratio, leading to a more compact tetranuclear core. Furthermore, the supramolecular architecture in (**I**) is reinforced by O—H···O hydrogen-bonding interactions and pronounced slipped π–π stacking between adjacent phenanthroline ligands, which contribute significantly to the packing. These combined structural features differentiate the title compound from the closest CSD analogues and highlight its enhanced connectivity and packing consolidation.

7. Synthesis and crystallization

3-Nitrophthalic acid (1.00 mmol, 0.211 g) was dissolved in *N*, *N*-dimethylformamide (DMF), 1,10-phenanthroline (1.00 mmol, 0.180 g) was dissolved in ethanol, and $Cu(CH_3COO)_2$ (1.00 mmol, 0.18 g) in distilled water. The mixture of solutions of 3-nitrophthalic acid and copper(II) acetate were combined in a flat-bottom flask and stirred for 20 min using a magnetic stirrer. The solution of 1,10-phenanthroline was added dropwise. The reaction mixture was stirred at 333 ± 0.5 K for an additional 20 min.

The resulting solution was left to stand at room temperature in a loosely covered vessel, maintaining a pH of approximately 6.0. After 12 days, blue prism-shaped crystals of (**I**) suitable for X-ray diffraction formed at the bottom of the vessel. The crystals were isolated by filtration.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were placed geometrically and refined using a riding model. One solvent-accessible region containing highly disordered electron density, probably corresponding to water molecule(s) of crystallization, could not be modelled satisfactorily. The contribution of this diffuse solvent was treated using the SQUEEZE procedure as implemented in *PLATON* (Spek, 2020). Three additional water molecules were located from difference-Fourier maps. However, their hydrogen atoms could not be positioned reliably due to unfavorable geometry and large displacement parameters. These hydrogen atoms were therefore omitted from the refinement. Hydrogen atoms attached to carbon atoms were placed in calculated positions and refined using a riding model.

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supporting information

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Crystal structure of a tetranuclear copper(II) complex with 1,10-phenanthroline and 3-nitrophthalate ligands

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Computing details

Tetrakis(*μ*-2-carboxy-6-nitrobenzoato-*κ*^{2}*O*:*O*′)bis(*μ*-3-nitrobenzene-1,2-dicarboxylato-*κ*^{2}*O*:*O*′)tetrakis[(1,10-phenanthroline-*κN*:*N*′)copper(II)] hexahydrate

Crystal data

$[Cu_4(C_8H_4NO_6)_4(C_8H_3NO_6)_2(C_{12}H_8N_2)_4]\cdot 6H_2O$
M_r = 2329.69
Monoclinic, *C*2/*c*
a = 24.890 (3) Å
b = 14.3705 (7) Å
c = 30.179 (3) Å
β = 116.919 (12)°
V = 9624.8 (17) Å^3
Z = 4
F(000) = 4720
D_x = 1.608 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 4168 reflections
θ = 3.6–60.4°
μ = 1.90 mm^{-1}
T = 293 K
Prism, blue
0.04 × 0.03 × 0.01 mm

Data collection

Xcalibur, Ruby diffractometer
ω scans
Absorption correction: multi-scan (CrysAlisPro; Agilent Technologies, 2014)
T_{min} = 0.916, T_{max} = 1.000
33685 measured reflections
9915 independent reflections
5785 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 77.0°, θ_{min} = 3.3°
h = −29→31
k = −14→17
l = −37→37
3 standard reflections every 100 reflections
intensity decay: 2.6%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.181
S = 1.01
9915 reflections
707 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 6.3715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.68380 (3)	0.40513 (4)	0.62556 (3)	0.0663 (2)
Cu2	0.57301 (3)	0.55106 (4)	0.58128 (3)	0.0681 (2)
O4	0.58184 (14)	0.41696 (19)	0.57240 (11)	0.0638 (7)
O5B	0.70341 (14)	0.47576 (19)	0.57949 (12)	0.0681 (8)
O4A	0.66823 (15)	0.5151 (2)	0.65655 (11)	0.0687 (8)
O6B	0.63082 (14)	0.5829 (2)	0.55696 (12)	0.0683 (8)
O3	0.49041 (16)	0.3972 (2)	0.50867 (13)	0.0779 (9)
O3A	0.76759 (18)	0.5158 (2)	0.70616 (15)	0.0917 (11)
N2	0.56699 (17)	0.6862 (2)	0.59599 (14)	0.0671 (9)
O5	0.49952 (19)	0.2586 (3)	0.58544 (15)	0.0955 (11)
N2A	0.65854 (18)	0.3142 (3)	0.66320 (13)	0.0700 (10)
N3	0.52032 (18)	0.5369 (3)	0.61551 (15)	0.0750 (11)
O4B	0.8250 (2)	0.5670 (4)	0.60462 (18)	0.1019 (13)
N3A	0.71965 (19)	0.2900 (3)	0.61278 (15)	0.0741 (10)
O1	0.5857 (2)	0.4276 (3)	0.47776 (14)	0.0961 (11)
O5A	0.75695 (19)	0.6524 (3)	0.63184 (16)	0.1052 (13)
O2B	0.8629 (2)	0.6170 (3)	0.5234 (2)	0.1107 (14)
O1A	0.6748 (2)	0.5141 (3)	0.75437 (17)	0.1106 (13)
N1B	0.8179 (3)	0.6167 (3)	0.4837 (2)	0.0887 (14)
O3B	0.8163 (2)	0.4526 (3)	0.5536 (2)	0.1175 (16)
O6	0.5031 (2)	0.1049 (3)	0.57957 (19)	0.1154 (15)
H6	0.487224	0.106557	0.598203	0.173*
C8B	0.6742 (2)	0.5460 (3)	0.55488 (16)	0.0617 (10)
N1A	0.6523 (3)	0.5930 (4)	0.74713 (19)	0.1032 (15)
C1	0.5413 (2)	0.3717 (3)	0.53517 (18)	0.0634 (11)
C2	0.5618 (2)	0.2773 (3)	0.52519 (17)	0.0654 (11)
C1A	0.7175 (3)	0.5513 (3)	0.68901 (19)	0.0707 (12)
C19A	0.7050 (2)	0.2121 (3)	0.63054 (18)	0.0701 (12)
C20A	0.6711 (2)	0.2256 (3)	0.65673 (16)	0.0687 (12)
C3B	0.6927 (2)	0.5888 (3)	0.51872 (17)	0.0644 (11)
C3	0.5471 (2)	0.1928 (3)	0.53959 (18)	0.0709 (12)
N1	0.6128 (3)	0.3575 (4)	0.4818 (2)	0.1069 (17)
C7B	0.7586 (2)	0.6211 (3)	0.48319 (19)	0.0703 (12)
C20	0.5331 (2)	0.7002 (3)	0.62056 (19)	0.0745 (13)
O1B	0.8192 (3)	0.6149 (4)	0.4437 (2)	0.1395 (19)
C2B	0.7503 (2)	0.5805 (3)	0.52163 (18)	0.0658 (11)
C1B	0.8005 (3)	0.5276 (4)	0.5624 (2)	0.0838 (15)
C12A	0.6527 (3)	0.1489 (3)	0.67555 (18)	0.0811 (15)
C4B	0.6482 (2)	0.6370 (3)	0.47936 (19)	0.0780 (13)

H4BA	0.610222	0.643114	0.477832	0.094*
C7	0.5951 (3)	0.2709 (3)	0.49873 (19)	0.0818 (14)
C2A	0.7119 (2)	0.6478 (3)	0.70521 (18)	0.0783 (14)
C8	0.5140 (2)	0.1911 (4)	0.5699 (2)	0.0809 (14)
C7A	0.6800 (3)	0.6674 (4)	0.7313 (2)	0.0872 (15)
C9	0.5893 (2)	0.7587 (3)	0.58342 (19)	0.0767 (13)
H9	0.612557	0.749391	0.566833	0.092*
C19	0.5086 (2)	0.6199 (4)	0.6313 (2)	0.0795 (14)
C15A	0.7218 (3)	0.1221 (4)	0.6232 (2)	0.0891 (16)
C3A	0.7410 (3)	0.7233 (4)	0.69456 (19)	0.0881 (16)
C6B	0.7145 (3)	0.6669 (3)	0.4439 (2)	0.0874 (16)
H6B	0.721880	0.691329	0.418653	0.105*
C9A	0.6260 (2)	0.3303 (4)	0.68692 (19)	0.0827 (14)
H9A	0.616953	0.391459	0.691125	0.099*
C18	0.4977 (3)	0.4609 (4)	0.6249 (2)	0.0906 (16)
H18	0.504946	0.404131	0.613777	0.109*
C10	0.5788 (3)	0.8502 (4)	0.5945 (2)	0.0933 (17)
H10	0.594584	0.900715	0.585008	0.112*
C5B	0.6590 (3)	0.6758 (4)	0.4427 (2)	0.0889 (16)
H5B	0.628610	0.708421	0.416909	0.107*
C4	0.5627 (3)	0.1082 (4)	0.5251 (2)	0.0892 (16)
H4	0.551056	0.052518	0.533840	0.107*
C13A	0.6694 (3)	0.0585 (4)	0.6670 (2)	0.105 (2)
H13	0.657078	0.006929	0.678589	0.126*
C12	0.5212 (3)	0.7884 (4)	0.6328 (2)	0.0962 (18)
C18A	0.7520 (3)	0.2806 (4)	0.5886 (3)	0.1020 (19)
H18A	0.762359	0.333169	0.576161	0.122*
C14A	0.7026 (3)	0.0453 (4)	0.6425 (2)	0.105 (2)
H14	0.713100	−0.014861	0.638137	0.126*
O6A	0.8244 (3)	0.7556 (4)	0.67908 (18)	0.176 (3)
O2A	0.6074 (3)	0.6095 (5)	0.7516 (3)	0.171 (3)
C10A	0.6049 (3)	0.2582 (5)	0.7059 (2)	0.1007 (19)
H10A	0.581844	0.271313	0.722211	0.121*
C6	0.6117 (3)	0.1874 (4)	0.4856 (2)	0.1042 (19)
H6C	0.634373	0.186840	0.468176	0.125*
C11A	0.6183 (3)	0.1689 (5)	0.7002 (2)	0.103 (2)
H11	0.604545	0.120620	0.712941	0.124*
C8A	0.7766 (3)	0.7104 (4)	0.6670 (2)	0.106 (2)
C5	0.5944 (3)	0.1058 (4)	0.4986 (2)	0.103 (2)
H5	0.604318	0.049097	0.489350	0.123*
C11	0.5460 (3)	0.8637 (4)	0.6189 (3)	0.105 (2)
H11A	0.539583	0.923959	0.626724	0.126*
C6A	0.6737 (4)	0.7582 (5)	0.7465 (2)	0.118 (2)
H6AA	0.650833	0.769487	0.763242	0.141*
C4A	0.7378 (4)	0.8113 (4)	0.7111 (2)	0.123 (3)
H4A	0.759020	0.860000	0.706021	0.147*
O2	0.6580 (4)	0.3537 (4)	0.4755 (3)	0.202 (3)
C16A	0.7568 (3)	0.1152 (4)	0.5989 (3)	0.118 (2)

H16	0.770545	0.057285	0.594687	0.141*
C15	0.4734 (3)	0.6262 (5)	0.6566 (3)	0.109 (2)
C17	0.4633 (3)	0.4621 (5)	0.6509 (3)	0.118 (2)
H17	0.448451	0.406855	0.657069	0.142*
C16	0.4519 (4)	0.5432 (5)	0.6668 (3)	0.132 (3)
H16A	0.429680	0.544244	0.684613	0.158*
C13	0.4841 (4)	0.7939 (5)	0.6585 (3)	0.138 (3)
H13A	0.475532	0.851723	0.667570	0.166*
C5A	0.7023 (4)	0.8275 (5)	0.7357 (3)	0.129 (3)
H5A	0.698483	0.888045	0.744745	0.155*
C17A	0.7712 (4)	0.1920 (5)	0.5811 (3)	0.128 (3)
H17A	0.793959	0.186844	0.563752	0.154*
C14	0.4620 (4)	0.7163 (6)	0.6695 (3)	0.143 (3)
H14A	0.438439	0.722208	0.686080	0.172*
O20W	0.4518 (2)	0.0830 (4)	0.6390 (2)	0.153 (2)
O22W	0.4510 (4)	0.2324 (7)	0.6994 (3)	0.235 (4)
O23W	0.8642 (4)	0.4422 (6)	0.6892 (3)	0.237 (4)
H4B	0.807 (3)	0.613 (4)	0.612 (2)	0.10 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0866 (5)	0.0514 (3)	0.0755 (4)	−0.0006 (3)	0.0495 (4)	0.0031 (3)
Cu2	0.0811 (4)	0.0560 (3)	0.0841 (5)	−0.0046 (3)	0.0524 (4)	−0.0123 (3)
O4	0.0750 (19)	0.0560 (16)	0.0661 (18)	−0.0035 (14)	0.0369 (16)	−0.0106 (14)
O5B	0.084 (2)	0.0547 (16)	0.083 (2)	0.0085 (14)	0.0531 (18)	0.0135 (15)
O4A	0.089 (2)	0.0560 (16)	0.0697 (19)	−0.0092 (15)	0.0436 (18)	−0.0073 (14)
O6B	0.076 (2)	0.0585 (16)	0.085 (2)	0.0074 (14)	0.0493 (18)	0.0046 (15)
O3	0.080 (2)	0.0674 (19)	0.079 (2)	0.0144 (16)	0.0293 (19)	−0.0058 (16)
O3A	0.090 (3)	0.069 (2)	0.103 (3)	0.0090 (19)	0.033 (2)	0.0103 (19)
N2	0.076 (2)	0.055 (2)	0.069 (2)	0.0011 (17)	0.032 (2)	−0.0082 (17)
O5	0.126 (3)	0.070 (2)	0.109 (3)	−0.017 (2)	0.069 (3)	−0.011 (2)
N2A	0.083 (3)	0.067 (2)	0.062 (2)	−0.0137 (19)	0.035 (2)	0.0017 (18)
N3	0.081 (3)	0.077 (3)	0.085 (3)	−0.011 (2)	0.053 (2)	−0.018 (2)
O4B	0.088 (3)	0.124 (4)	0.098 (3)	0.005 (3)	0.047 (3)	0.023 (3)
N3A	0.089 (3)	0.060 (2)	0.084 (3)	0.0082 (19)	0.048 (2)	0.0077 (19)
O1	0.139 (4)	0.076 (2)	0.087 (3)	0.010 (2)	0.063 (3)	0.0061 (19)
O5A	0.111 (3)	0.096 (3)	0.097 (3)	−0.032 (2)	0.037 (2)	−0.013 (2)
O2B	0.111 (3)	0.101 (3)	0.154 (4)	0.000 (3)	0.090 (3)	0.010 (3)
O1A	0.145 (4)	0.103 (3)	0.101 (3)	−0.011 (3)	0.071 (3)	−0.001 (3)
N1B	0.125 (4)	0.056 (2)	0.126 (4)	−0.002 (3)	0.093 (4)	0.004 (3)
O3B	0.131 (4)	0.080 (2)	0.189 (5)	0.038 (2)	0.115 (4)	0.039 (3)
O6	0.113 (3)	0.070 (2)	0.176 (5)	−0.006 (2)	0.077 (3)	0.018 (3)
C8B	0.071 (3)	0.055 (2)	0.068 (3)	−0.001 (2)	0.039 (2)	0.001 (2)
N1A	0.113 (4)	0.121 (4)	0.082 (3)	0.007 (4)	0.050 (3)	−0.016 (3)
C1	0.075 (3)	0.052 (2)	0.071 (3)	0.001 (2)	0.039 (3)	−0.004 (2)
C2	0.071 (3)	0.057 (2)	0.063 (3)	0.005 (2)	0.026 (2)	−0.0066 (19)
C1A	0.091 (4)	0.056 (2)	0.072 (3)	−0.002 (3)	0.042 (3)	0.004 (2)

C19A	0.079 (3)	0.049 (2)	0.068 (3)	0.001 (2)	0.021 (2)	0.005 (2)
C20A	0.081 (3)	0.060 (3)	0.055 (2)	−0.007 (2)	0.022 (2)	0.005 (2)
C3B	0.084 (3)	0.051 (2)	0.068 (3)	0.002 (2)	0.043 (2)	0.003 (2)
C3	0.070 (3)	0.056 (2)	0.074 (3)	0.005 (2)	0.021 (2)	−0.008 (2)
N1	0.162 (5)	0.088 (3)	0.113 (4)	0.012 (3)	0.100 (4)	0.001 (3)
C7B	0.099 (4)	0.053 (2)	0.082 (3)	−0.004 (2)	0.061 (3)	−0.004 (2)
C20	0.075 (3)	0.077 (3)	0.080 (3)	−0.001 (2)	0.043 (3)	−0.019 (2)
O1B	0.196 (5)	0.144 (4)	0.154 (4)	−0.003 (4)	0.146 (4)	−0.001 (3)
C2B	0.088 (3)	0.048 (2)	0.078 (3)	0.003 (2)	0.052 (3)	0.003 (2)
C1B	0.089 (4)	0.084 (4)	0.103 (4)	0.002 (3)	0.065 (4)	0.019 (3)
C12A	0.098 (4)	0.069 (3)	0.056 (3)	−0.022 (3)	0.017 (3)	0.006 (2)
C4B	0.091 (4)	0.067 (3)	0.082 (3)	0.001 (3)	0.045 (3)	0.009 (2)
C7	0.105 (4)	0.069 (3)	0.076 (3)	0.015 (3)	0.045 (3)	−0.004 (2)
C2A	0.096 (4)	0.064 (3)	0.057 (3)	0.004 (3)	0.020 (3)	−0.003 (2)
C8	0.068 (3)	0.063 (3)	0.095 (4)	−0.009 (2)	0.023 (3)	0.003 (3)
C7A	0.098 (4)	0.076 (3)	0.069 (3)	−0.001 (3)	0.021 (3)	−0.008 (3)
C9	0.085 (3)	0.064 (3)	0.084 (3)	0.002 (2)	0.040 (3)	0.001 (2)
C19	0.089 (3)	0.082 (3)	0.083 (3)	−0.011 (3)	0.053 (3)	−0.027 (3)
C15A	0.103 (4)	0.061 (3)	0.084 (4)	0.009 (3)	0.025 (3)	−0.001 (3)
C3A	0.110 (4)	0.067 (3)	0.061 (3)	−0.016 (3)	0.015 (3)	0.001 (2)
C6B	0.134 (5)	0.066 (3)	0.079 (3)	−0.001 (3)	0.063 (4)	0.007 (3)
C9A	0.099 (4)	0.085 (3)	0.078 (3)	−0.013 (3)	0.052 (3)	−0.001 (3)
C18	0.108 (4)	0.084 (4)	0.105 (4)	−0.019 (3)	0.071 (4)	−0.017 (3)
C10	0.109 (4)	0.060 (3)	0.116 (5)	−0.002 (3)	0.056 (4)	−0.006 (3)
C5B	0.110 (4)	0.081 (3)	0.071 (3)	−0.001 (3)	0.037 (3)	0.014 (3)
C4	0.085 (4)	0.063 (3)	0.102 (4)	0.007 (3)	0.027 (3)	−0.006 (3)
C13A	0.140 (6)	0.063 (3)	0.081 (4)	−0.022 (3)	0.023 (4)	0.010 (3)
C12	0.101 (4)	0.079 (4)	0.118 (5)	−0.005 (3)	0.058 (4)	−0.037 (3)
C18A	0.122 (5)	0.078 (3)	0.142 (5)	0.012 (3)	0.090 (5)	0.010 (3)
C14A	0.137 (6)	0.056 (3)	0.094 (4)	0.010 (3)	0.029 (4)	0.009 (3)
O6A	0.225 (6)	0.207 (6)	0.098 (3)	−0.142 (5)	0.074 (4)	−0.034 (4)
O2A	0.159 (5)	0.214 (7)	0.194 (6)	0.015 (5)	0.128 (5)	−0.011 (5)
C10A	0.118 (5)	0.112 (5)	0.084 (4)	−0.035 (4)	0.056 (4)	−0.007 (3)
C6	0.131 (5)	0.091 (4)	0.106 (4)	0.026 (4)	0.067 (4)	−0.016 (3)
C11A	0.122 (5)	0.111 (5)	0.073 (4)	−0.036 (4)	0.041 (4)	0.007 (3)
C8A	0.151 (6)	0.091 (4)	0.068 (3)	−0.041 (4)	0.041 (4)	0.003 (3)
C5	0.118 (5)	0.069 (3)	0.113 (5)	0.021 (3)	0.045 (4)	−0.020 (3)
C11	0.111 (5)	0.072 (4)	0.131 (5)	0.007 (3)	0.054 (4)	−0.026 (4)
C6A	0.145 (6)	0.097 (5)	0.085 (4)	0.023 (4)	0.029 (4)	−0.024 (4)
C4A	0.172 (7)	0.056 (3)	0.081 (4)	−0.002 (4)	0.005 (4)	0.001 (3)
O2	0.304 (9)	0.134 (4)	0.322 (9)	0.032 (5)	0.277 (8)	0.016 (5)
C16A	0.149 (6)	0.073 (4)	0.143 (6)	0.035 (4)	0.077 (5)	0.007 (4)
C15	0.124 (5)	0.115 (5)	0.125 (5)	−0.016 (4)	0.088 (5)	−0.046 (4)
C17	0.138 (6)	0.119 (5)	0.142 (6)	−0.036 (4)	0.103 (5)	−0.026 (5)
C16	0.165 (7)	0.139 (6)	0.157 (7)	−0.046 (5)	0.130 (6)	−0.055 (5)
C13	0.152 (7)	0.116 (6)	0.183 (8)	−0.010 (5)	0.107 (6)	−0.074 (6)
C5A	0.173 (8)	0.067 (4)	0.098 (5)	0.015 (4)	0.017 (5)	−0.022 (4)
C17A	0.155 (7)	0.098 (5)	0.183 (8)	0.023 (4)	0.123 (6)	0.000 (5)

C14	0.170 (8)	0.131 (6)	0.194 (8)	−0.031 (5)	0.140 (7)	−0.066 (6)
O20W	0.104 (4)	0.193 (5)	0.160 (5)	−0.027 (3)	0.057 (3)	0.042 (4)
O22W	0.218 (8)	0.310 (10)	0.242 (8)	−0.020 (7)	0.163 (7)	−0.008 (7)
O23W	0.231 (8)	0.298 (10)	0.239 (8)	0.104 (7)	0.156 (7)	0.163 (7)

Geometric parameters (Å, º)

Cu1—O5B	1.953 (3)	C12A—C11A	1.396 (8)
Cu1—O4A	1.962 (3)	C12A—C13A	1.423 (8)
Cu1—N3A	1.999 (4)	C4B—C5B	1.370 (7)
Cu1—N2A	2.009 (4)	C4B—H4BA	0.9300
Cu1—O4	2.314 (3)	C7—C6	1.384 (7)
Cu2—O6B	1.944 (3)	C2A—C7A	1.377 (8)
Cu2—O4	1.972 (3)	C2A—C3A	1.419 (7)
Cu2—N2	2.013 (4)	C7A—C6A	1.415 (8)
Cu2—N3	2.014 (4)	C9—C10	1.411 (7)
Cu2—O4A	2.484 (3)	C9—H9	0.9300
O4—C1	1.295 (5)	C19—C15	1.405 (7)
O5B—C8B	1.269 (5)	C15A—C16A	1.375 (9)
O4A—C1A	1.283 (6)	C15A—C14A	1.428 (9)
O6B—C8B	1.229 (5)	C3A—C4A	1.375 (8)
O3—C1	1.210 (5)	C3A—C8A	1.476 (9)
O3A—C1A	1.224 (6)	C6B—C5B	1.370 (8)
N2—C9	1.315 (6)	C6B—H6B	0.9300
N2—C20	1.367 (6)	C9A—C10A	1.396 (7)
O5—C8	1.201 (6)	C9A—H9A	0.9300
N2A—C9A	1.321 (6)	C18—C17	1.399 (8)
N2A—C20A	1.347 (6)	C18—H18	0.9300
N3—C18	1.316 (6)	C10—C11	1.337 (8)
N3—C19	1.364 (6)	C10—H10	0.9300
O4B—C1B	1.269 (7)	C5B—H5B	0.9300
O4B—H4B	0.88 (6)	C4—C5	1.352 (8)
N3A—C18A	1.317 (7)	C4—H4	0.9300
N3A—C19A	1.360 (6)	C13A—C14A	1.345 (9)
O1—N1	1.188 (6)	C13A—H13	0.9300
O5A—C8A	1.261 (7)	C12—C11	1.402 (9)
O2B—N1B	1.216 (7)	C12—C13	1.452 (9)
O1A—N1A	1.240 (6)	C18A—C17A	1.414 (8)
N1B—O1B	1.220 (6)	C18A—H18A	0.9300
N1B—C7B	1.471 (7)	C14A—H14	0.9300
O3B—C1B	1.218 (6)	O6A—C8A	1.256 (8)
O6—C8	1.328 (6)	C10A—C11A	1.356 (9)
O6—H6	0.8200	C10A—H10A	0.9300
C8B—C3B	1.496 (6)	C6—C5	1.367 (9)
N1A—O2A	1.207 (7)	C6—H6C	0.9300
N1A—C7A	1.465 (8)	C11A—H11	0.9300
C1—C2	1.526 (6)	C5—H5	0.9300
C2—C7	1.391 (7)	C11—H11A	0.9300

C2—C3	1.394 (6)	C6A—C5A	1.349 (11)
C1A—C2A	1.499 (7)	C6A—H6AA	0.9300
C19A—C15A	1.407 (7)	C4A—C5A	1.406 (11)
C19A—C20A	1.405 (7)	C4A—H4A	0.9300
C20A—C12A	1.408 (6)	C16A—C17A	1.347 (9)
C3B—C4B	1.388 (7)	C16A—H16	0.9300
C3B—C2B	1.401 (6)	C15—C16	1.396 (9)
C3—C4	1.406 (7)	C15—C14	1.417 (9)
C3—C8	1.483 (8)	C17—C16	1.339 (9)
N1—O2	1.225 (7)	C17—H17	0.9300
N1—C7	1.485 (7)	C16—H16A	0.9300
C7B—C6B	1.366 (7)	C13—C14	1.350 (10)
C7B—C2B	1.395 (6)	C13—H13A	0.9300
C20—C12	1.388 (7)	C5A—H5A	0.9300
C20—C19	1.409 (7)	C17A—H17A	0.9300
C2B—C1B	1.504 (7)	C14—H14A	0.9300

O5B—Cu1—O4A	95.02 (12)	O6—C8—C3	112.1 (5)
O5B—Cu1—N3A	90.89 (14)	C2A—C7A—C6A	123.5 (6)
O4A—Cu1—N3A	163.85 (16)	C2A—C7A—N1A	121.1 (5)
O5B—Cu1—N2A	169.40 (14)	C6A—C7A—N1A	115.4 (6)
O4A—Cu1—N2A	94.28 (15)	N2—C9—C10	121.5 (5)
N3A—Cu1—N2A	81.49 (16)	N2—C9—H9	119.3
O5B—Cu1—O4	90.99 (12)	C10—C9—H9	119.3
O4A—Cu1—O4	83.11 (12)	N3—C19—C15	122.1 (5)
N3A—Cu1—O4	111.85 (15)	N3—C19—C20	117.0 (4)
N2A—Cu1—O4	85.08 (14)	C15—C19—C20	120.9 (5)
O6B—Cu2—O4	91.81 (12)	C16A—C15A—C19A	117.1 (5)
O6B—Cu2—N2	89.88 (14)	C16A—C15A—C14A	125.0 (6)
O4—Cu2—N2	175.61 (14)	C19A—C15A—C14A	117.9 (6)
O6B—Cu2—N3	169.52 (15)	C4A—C3A—C2A	120.1 (7)
O4—Cu2—N3	96.28 (14)	C4A—C3A—C8A	117.9 (6)
N2—Cu2—N3	81.59 (16)	C2A—C3A—C8A	122.0 (5)
C1—O4—Cu2	121.2 (3)	C7B—C6B—C5B	118.2 (5)
C1—O4—Cu1	138.0 (3)	C7B—C6B—H6B	120.9
Cu2—O4—Cu1	97.60 (12)	C5B—C6B—H6B	120.9
C8B—O5B—Cu1	124.6 (3)	N2A—C9A—C10A	121.9 (5)
C1A—O4A—Cu1	111.3 (3)	N2A—C9A—H9A	119.1
C8B—O6B—Cu2	137.3 (3)	C10A—C9A—H9A	119.0
C9—N2—C20	119.0 (4)	N3—C18—C17	122.7 (5)
C9—N2—Cu2	128.1 (3)	N3—C18—H18	118.7
C20—N2—Cu2	112.8 (3)	C17—C18—H18	118.7
C9A—N2A—C20A	118.9 (4)	C11—C10—C9	119.4 (6)
C9A—N2A—Cu1	128.1 (4)	C11—C10—H10	120.3
C20A—N2A—Cu1	112.3 (3)	C9—C10—H10	120.3
C18—N3—C19	118.1 (4)	C4B—C5B—C6B	120.3 (5)
C18—N3—Cu2	129.4 (3)	C4B—C5B—H5B	119.9
C19—N3—Cu2	112.4 (3)	C6B—C5B—H5B	119.9

C1B—O4B—H4B	121 (4)	C5—C4—C3	121.6 (6)
C18A—N3A—C19A	118.4 (4)	C5—C4—H4	119.2
C18A—N3A—Cu1	129.1 (4)	C3—C4—H4	119.2
C19A—N3A—Cu1	112.5 (3)	C14A—C13A—C12A	122.1 (6)
O2B—N1B—O1B	123.4 (6)	C14A—C13A—H13	119.0
O2B—N1B—C7B	118.8 (5)	C12A—C13A—H13	119.0
O1B—N1B—C7B	117.8 (6)	C20—C12—C11	116.7 (5)
C8—O6—H6	109.5	C20—C12—C13	117.1 (6)
O6B—C8B—O5B	126.7 (4)	C11—C12—C13	126.2 (6)
O6B—C8B—C3B	115.3 (4)	N3A—C18A—C17A	121.2 (6)
O5B—C8B—C3B	118.0 (4)	N3A—C18A—H18A	119.4
O2A—N1A—O1A	121.8 (7)	C17A—C18A—H18A	119.4
O2A—N1A—C7A	119.3 (6)	C13A—C14A—C15A	121.1 (6)
O1A—N1A—C7A	118.9 (5)	C13A—C14A—H14	119.5
O3—C1—O4	126.3 (4)	C15A—C14A—H14	119.5
O3—C1—C2	118.8 (4)	C11A—C10A—C9A	119.4 (6)
O4—C1—C2	114.8 (4)	C11A—C10A—H10A	120.3
C7—C2—C3	115.5 (4)	C9A—C10A—H10A	120.3
C7—C2—C1	120.7 (4)	C5—C6—C7	119.3 (6)
C3—C2—C1	123.7 (4)	C5—C6—H6C	120.4
O3A—C1A—O4A	126.4 (5)	C7—C6—H6C	120.4
O3A—C1A—C2A	118.4 (5)	C10A—C11A—C12A	120.5 (5)
O4A—C1A—C2A	115.2 (5)	C10A—C11A—H11	119.8
N3A—C19A—C15A	122.9 (5)	C12A—C11A—H11	119.8
N3A—C19A—C20A	116.4 (4)	O6A—C8A—O5A	122.8 (7)
C15A—C19A—C20A	120.7 (5)	O6A—C8A—C3A	120.2 (6)
N2A—C20A—C19A	116.7 (4)	O5A—C8A—C3A	117.0 (6)
N2A—C20A—C12A	122.8 (5)	C4—C5—C6	119.4 (5)
C19A—C20A—C12A	120.4 (5)	C4—C5—H5	120.3
C4B—C3B—C2B	119.5 (4)	C6—C5—H5	120.3
C4B—C3B—C8B	116.1 (4)	C10—C11—C12	120.9 (5)
C2B—C3B—C8B	124.3 (4)	C10—C11—H11A	119.5
C2—C3—C4	120.5 (5)	C12—C11—H11A	119.5
C2—C3—C8	120.3 (4)	C5A—C6A—C7A	117.0 (7)
C4—C3—C8	119.3 (5)	C5A—C6A—H6AA	121.5
O1—N1—O2	122.7 (6)	C7A—C6A—H6AA	121.5
O1—N1—C7	120.2 (5)	C3A—C4A—C5A	119.8 (7)
O2—N1—C7	117.0 (5)	C3A—C4A—H4A	120.1
C6B—C7B—C2B	124.1 (5)	C5A—C4A—H4A	120.1
C6B—C7B—N1B	116.0 (5)	C17A—C16A—C15A	120.2 (6)
C2B—C7B—N1B	120.0 (5)	C17A—C16A—H16	119.9
N2—C20—C12	122.5 (5)	C15A—C16A—H16	119.9
N2—C20—C19	116.1 (4)	C16—C15—C19	117.4 (5)
C12—C20—C19	121.4 (5)	C16—C15—C14	125.2 (6)
C7B—C2B—C3B	116.4 (4)	C19—C15—C14	117.4 (6)
C7B—C2B—C1B	120.8 (4)	C16—C17—C18	119.7 (6)
C3B—C2B—C1B	122.7 (4)	C16—C17—H17	120.2
O3B—C1B—O4B	124.0 (6)	C18—C17—H17	120.2

O3B—C1B—C2B	119.9 (6)	C17—C16—C15	120.0 (6)
O4B—C1B—C2B	116.1 (5)	C17—C16—H16A	120.0
C11A—C12A—C20A	116.4 (5)	C15—C16—H16A	120.0
C11A—C12A—C13A	125.9 (6)	C14—C13—C12	121.1 (6)
C20A—C12A—C13A	117.8 (6)	C14—C13—H13A	119.5
C5B—C4B—C3B	121.5 (5)	C12—C13—H13A	119.5
C5B—C4B—H4BA	119.3	C6A—C5A—C4A	122.2 (6)
C3B—C4B—H4BA	119.3	C6A—C5A—H5A	118.9
C6—C7—C2	123.7 (5)	C4A—C5A—H5A	118.9
C6—C7—N1	117.0 (5)	C16A—C17A—C18A	120.2 (6)
C2—C7—N1	119.3 (4)	C16A—C17A—H17A	119.9
C7A—C2A—C3A	117.3 (5)	C18A—C17A—H17A	119.9
C7A—C2A—C1A	122.6 (5)	C13—C14—C15	122.1 (6)
C3A—C2A—C1A	120.1 (5)	C13—C14—H14A	118.9
O5—C8—O6	122.7 (6)	C15—C14—H14A	118.9
O5—C8—C3	125.1 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6···O20*W*	0.82	1.84	2.649 (7)	168
C9—H9···O6*B*	0.93	2.48	2.972 (6)	113
C9*A*—H9*A*···O1*A*	0.93	2.52	3.217 (7)	132
C18—H18···O5	0.93	2.24	3.150 (7)	166
C18*A*—H18*A*···O5*B*	0.93	2.55	3.017 (6)	112
C18*A*—H18*A*···O3*B*	0.93	2.46	3.365 (7)	165
C6—H6*C*···O3*B*^{i}	0.93	2.58	3.252 (7)	129
C17*A*—H17*A*···O2^{i}	0.93	2.11	3.027 (8)	169
O4*B*—H4*B*···O5*A*	0.88 (6)	1.70 (6)	2.512 (7)	151 (6)

Symmetry code: (i) −*x*+3/2, −*y*+1/2, −*z*+1.