Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis and crystal structure of a new tetranuclear copper(II) complex based on the Schiff base (*E*)-2-[(2-hydroxy-5-methoxybenzylidene)-amino]benzoic acid

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Received 19 May 2026
Accepted 26 May 2026

Edited by X. Hao, Institute of Chemistry, Chinese Academy of Sciences

Keywords: crystal structure; tetranuclear copper complex; Schiff base ligand.

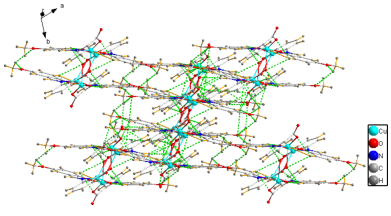
CCDC reference: 2544733

Supporting information: this article has supporting information at journals.iucr.org/e

The title complex, bis{μ_4-(*E*)-2-[(5-methoxy-2-oxidobenzylidene)amino]-benzoato}bis{μ_2-(*E*)-2-[(5-methoxy-2-oxidobenzylidene)amino]benzoato}tetra-copper(II), $[Cu_4(C_{15}H_{11}NO_4)_4]$ or $Cu_4(L)_4$, was synthesized by the solvothermal reaction of (*E*)-2-[(2-hydroxy-5-methoxybenzylidene)amino]benzoic acid (H_2L) with copper(II) chloride. It crystallizes in the triclinic system with space group $P\bar{1}$. The tetranuclear structure consists of two fully symmetric dinuclear copper moieties. In the dinuclear copper structural unit, both copper(II) metal centers exhibit a five-coordinate NO_4 environment. Of the four coordinating oxygen atoms, two are phenolate oxygen atoms acting as bridges from two different ligands, while the other two oxygen atoms are derived from the carboxyl groups of two distinct ligands, respectively. *SHAPE* analysis indicates that both copper(II) centers adopt a distorted trigonal–bipyramidal (D_{3h}) geometry. C—H···O hydrogen bonds and C—H···π interactions contribute to the cohesion of the crystal packing.

1. Chemical context

Coordination polymers constructed from Schiff base ligands bearing phenolic hydroxyl and carboxyl groups have attracted extensive research interest, owing to their elegant structural topologies and fascinating magnetic properties (Allendorf *et al.*, 2009; Karahan *et al.*, 2015). Such ligands are distinguished by facile synthesis, flexible structural modification, and strong coordination capability (Zhang *et al.*, 2012). In particular, the corresponding metal complexes are easily accessible, feature diversifiable and tunable structures, and possess desirable magnetic behaviors as well as biological activities (Karahan *et al.*, 2015). The rational design of building blocks, together with the utilization of coordination bonds and non-covalent interactions to self-assemble multidimensional supramolecular aggregates with delicate architectures for potential functional material applications, represents a vital research hotspot in supramolecular chemistry and crystal engineering (Sasmal *et al.*, 2011). In light of the above, this paper reports the synthesis and crystal structure of the title complex.



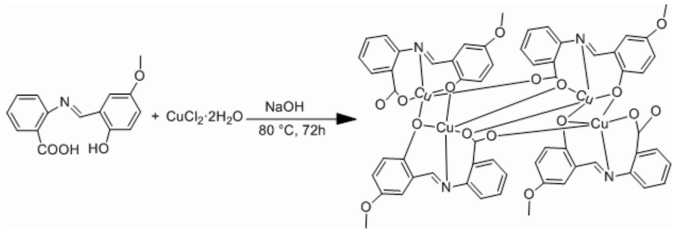


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O6	0.93	2.55	3.112 (3)	119
C29—H29···O2	0.93	2.28	2.945 (2)	128
C23—H23···O5^{i}	0.93	2.58	3.432 (2)	153
C27—H27A···O5^{ii}	0.96	2.63	3.567 (3)	165

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

2. Structural commentary

The title $Cu_4(L)_4$ complex crystallizes in the triclinic crystal system in space group $P\overline{1}$. The tetranuclear structural motif is constructed from two symmetry-equivalent dinuclear Cu^{II} subunits bridged by phenolic hydroxyl and carboxylate groups (Fig. 1). In the dinuclear Cu^{II} unit, each central divalent copper ion adopts a five-coordinate configuration and displays a distorted trigonal–bipyramidal (D_{3h}) geometry (Fig. 2). Within the coordination polyhedron of each Cu^{II} center, the coordinating atoms consist of one nitrogen atom (N1), one carboxylate oxygen atom (O2) and one phenolate oxygen atom (O3) all originating from a single ligand, one carboxylate oxygen atom (O2A) from a second ligand, and one phenolate oxygen atom (O7) from a third ligand. In general, five-coordinate Cu^{II} ions are typically tend to adopt square-pyramidal coordination geometries. The distinctive distorted trigonal–bipyramidal coordination environment of the Cu^{II} atom in the title complex is mainly induced by the inherent steric hindrance of the ligand framework, and intramolecular hydrogen-bonding interactions (Table 1) further contribute to the structural stabilization. The two dinuclear Cu^{II} cores form an approximately square-planar arrangement. Two such nearly square dinuclear moieties are further interconnected *via* two carboxylate oxygen bridges, affording a zigzag chain-shaped three-fused cyclic architecture (Fig. 3). For the four Cu^{II} centers, the adjacent Cu···Cu interatomic distances are 3.0091 (3), 3.6310 (4) and 3.0091 (3) Å. The Cu—N bond lengths are 1.9530 (14) and 1.9295 (15) Å, while the Cu—O bond distances are in the range 1.8810 (12) to 2.3276 (14) Å. A continuous shape analysis of the coordination geometries for the two Cu^{II} centers within the dinuclear fragment was performed by means of the *SHAPE 2.0* program (Llunell *et al.*, 2013), and the corresponding quantitative parameters are summarized in Table 2.

Table 2
Agreement factor between the coordination polyhedron of the Cu^{II} ion in complex **1** and the various ideal polyhedra calculated by the *SHAPE* program.

Atom	PP-5 (D_{5h})	vOC-5 (C_{4v})	TBPY-5 (D_{3h})	SPY-5 (C_{4v})	JTBPY-5 (D_{3h})
Cu1	21.750	7.133	6.260	6.286	10.635
Cu2	29.860	4.817	1.702	3.670	5.327

PP-5 (D_{5h}): pentagon; vOC-5 (C_{4v}) vacant octahedron; TBPY-5 (D_{3h}): trigonal bipyramid; SPY-5 (C_{4v}): spherical square pyramid; JTBPY-5 (D_{3h}): Johnson trigonal bipyramid J12.

3. Supramolecular features

In the crystal, weak C—H···O hydrogen bonds and C—H···π interactions interconnect the complex molecules to construct a three-dimensional supramolecular network (Fig. 4, Table 1).

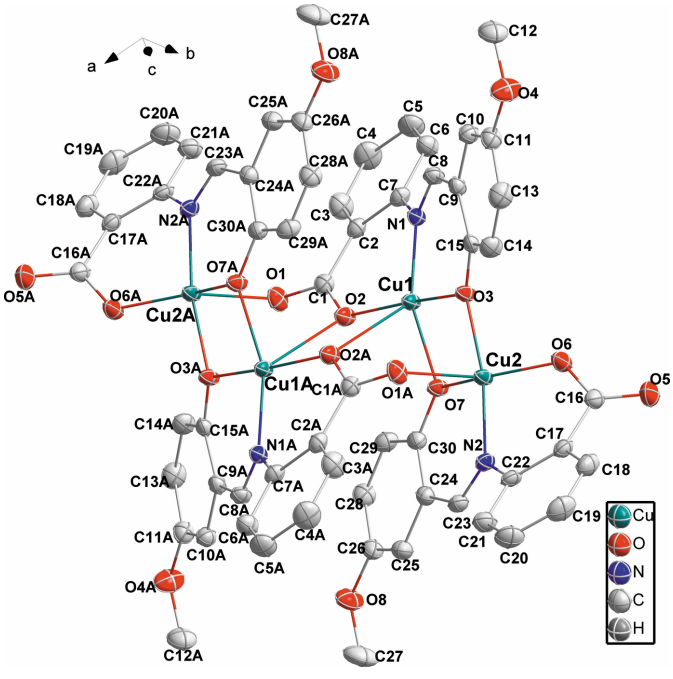


Figure 1
Molecular structure of the title compound with 50% probability ellipsoids. For clarity, H atoms are not shown.

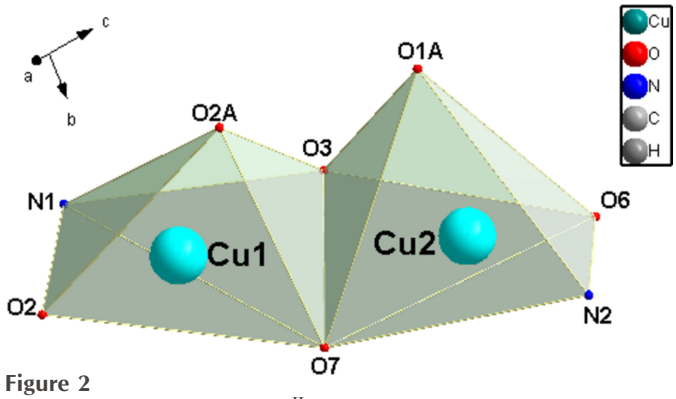


Figure 2
Coordination polyhedra of Cu^{II} ions. Colour: cyan (Cu), red (O), blue (N).

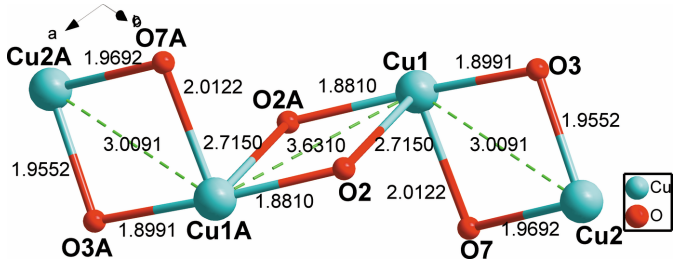


Figure 3
Zigzag chain configuration in the complex.

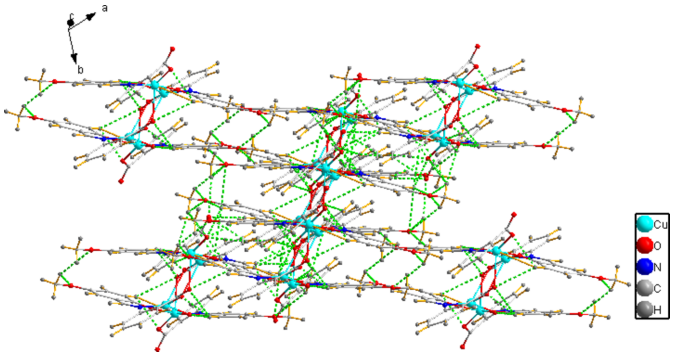


Figure 4
The crystal packing with the C—H···O hydrogen bonds shown as green dashed lines.

4. Database survey

A search was performed using the Cambridge Structural Database (CSD, Version 5.37, Update 1; Groom *et al.*, 2016) to retrieve linear tetranuclear copper(II) complexes constructed from Schiff base ligands structurally analogous to the title compound. Only few related crystal structures were identified: the complex [Cu(salpd-μ-O,O′)(μ-*L*)Cu(μ-CH_3O)$_2$Cu(μ-*L*)salpd-μ-O,*O*′)Cu], (*L* = acetate or formate ions) (KEPZAG; Fukuhara *et al.*, 1989); a series of linear tetranuclear copper(II) complexes [Cu_4(bzacpro)$_2$(C_2H_5O)$_2$], [Cu_4(bzacbu)$_2$(CH_3O)$_2$], [Cu_4(bzacpen)$_2$(CH_3CO_2)$_2$], and [Cu_4(bzacpen)$_2$O]·H_2O·(*N*,*N*′-bis(1-methyl-3-hydroxy-3-phenyl-2-propen-1-ylidene)-1,3-diamino-2-propanol (H_3bzacpro), *N*,*N*′-bis(1-methyl-3-hydroxy-3-phenyl-2-propen-1-ylidene)-1,4-diamino-2-butanol (H_3bzacbu), and *N*,*N*′-bis(1-methyl-3-hydroxy-3-phenyl-2-propen-1-ylidene)-1,5-diamino-3-pentanol (H_3bzacpen) (EHUPEC, EHUPOM, EHUPUS and EHUQAZ; Mikuriya *et al.*, 2002); the complex [Cu_4(2,2′-bpy)$_6$(ip)$_2$(H_2O)$_2$]·4ClO_4·6H_2O (2,2′-bpy = 2,2′-bipyridine and H_2ip = isophthalic acid) (CCDC 661868; Zhang *et al.*, 2011). Among the six linear tetranuclear copper(II) aggregates reported in their work, the Cu—O and Cu—N bond lengths at each coordination site are well consistent with those of the title compound in this study. In addition, two linear tetranuclear copper(II) complexes, formulated as [Cu_4(L_1)$_2$(μ-N_3)$_2$(N_3)$_2$] (**1**) and [Cu_4(L_2)$_2$(μ-N_3)$_2$(N_3)$_2$] (**2**). [L_1= *N*,*N*′-bis-(salicylidene)diaminopropane (salpn) and L_2=*N*,*N*′-bis-(salicylidene)diaminobenzene (salophen)] (AGEZAQ and AGEZEU; Pandey *et al.*, 2018). These two linear tetranuclear copper(II) species share a fundamental structural framework identical to that of the title compound.

5. Synthesis and crystallization

A mixture of $CuCl_2$·2H_2O (0.05 mmol), the ligand H_2L (0.05 mmol) and NaOH (0.1 mmol) was placed into a Pyrex tube (about 12 mL) together with ethanol (2 mL) and deionized water (2 mL). The sealed tube was heated at 353 K under autogenous pressure for 72 h. Dark-green elongated crystals suitable for single-crystal X-ray diffraction analysis were successfully obtained. Based on copper, the yield of the title complex was calculated to be 56% (0.009 g).

Table 3
Experimental details.

Crystal data	
Chemical formula	[Cu_4($C_{15}H_{11}NO_4$)$_4$]
M_r	1331.15
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	10.7949 (6), 11.0214 (6), 11.9680 (6)
α, β, γ (°)	103.651 (2), 95.318 (2), 109.881 (2)
V (Å^3)	1277.69 (12)
Z	1
Radiation type	Mo *K*α
μ (mm^{-1})	1.73
Crystal size (mm)	0.44 × 0.42 × 0.26
Data collection	
Diffractometer	Bruker CCD area detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.546, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	48410, 5891, 5107
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.026, 0.069, 1.03
No. of reflections	5891
No. of parameters	381
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.44

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C—H hydrogen atoms were generated at idealized geometrical positions, with methyl hydrogen atoms allowed to rotate while remaining non-tilting. These hydrogen atoms were refined isotropically under the thermal constraint: U_{iso}(H)=1.2U_{eq}(C) (1.5U_{eq}(C) for methyl hydrogen atoms).

Acknowledgements

We sincerely acknowledge the financial and material support from the Henan Provincial Natural Science Foundation Committee, the Department of Education of Henan Province, Zhengzhou Normal University, and the College of Chemistry and Chemical Engineering.

Funding information

Funding for this research was provided by: the Henan Provincial Science and Technology Research Program (grant No. 252102230022); Henan Provincial Natural Science Foundation (grant Nos. 262300420620, 262300422366); the Key Scientific Research Projects of Colleges and Universities in Henan Province (grant No. 25B150030); startup funding from

Zhengzhou Normal University (grant No. ZZNUKY00001, 12345644444); College Students' innovation and entrepreneurship training program of Henan (scholarship No. S202512949018); College Students' innovation and entrepreneurship training program of Zhengzhou Normal University (scholarship No. DCY2024028).

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supporting information

Acta Cryst. (2026). E**82** [https://doi.org/10.1107/S2056989026005554]

Synthesis and crystal structure of a new tetranuclear copper(II) complex based on the Schiff base (*E*)-2-[(2-hydroxy-5-methoxybenzylidene)amino]benzoic acid

Dawei Li, Wanying Qi, Jingjing Wang, Haiyang Dong, Kuilin Lv and Kaige Shi

Computing details

Bis{μ_4-(*E*)-2-[(5-methoxy-2-oxidobenzylidene)amino]benzoato}bis{μ_2-(*E*)-2-[(5-methoxy-2-oxidobenzylidene)amino]benzoato}tetracopper(II)

Crystal data

$[Cu_4(C_{15}H_{11}NO_4)_4]$
M_r = 1331.15
Triclinic, $P\overline{1}$
a = 10.7949 (6) Å
b = 11.0214 (6) Å
c = 11.9680 (6) Å
α = 103.651 (2)°
β = 95.318 (2)°
γ = 109.881 (2)°
V = 1277.69 (12) Å^3
Z = 1
$F(000)$ = 676
D_x = 1.730 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9991 reflections
θ = 2.4–27.5°
μ = 1.73 mm^{-1}
T = 296 K
Block, dull greenish blue
0.44 × 0.42 × 0.26 mm

Data collection

Bruker CCD area detector diffractometer
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.546, T_{max} = 0.746
48410 measured reflections
5891 independent reflections
5107 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.6°, θ_{min} = 2.4°
h = −14→14
k = −14→14
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.03
5891 reflections
381 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 0.9769P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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	0.64016 (2)	0.44708 (2)	0.52175 (2)	0.01786 (6)
Cu2	0.63788 (2)	0.31527 (2)	0.27047 (2)	0.01985 (7)
O7	0.52279 (12)	0.28733 (12)	0.38781 (10)	0.0202 (3)
O3	0.75631 (12)	0.45024 (13)	0.41168 (10)	0.0196 (3)
O2	0.50759 (12)	0.46228 (13)	0.60953 (11)	0.0227 (3)
O1	0.41991 (13)	0.51054 (14)	0.76564 (11)	0.0254 (3)
O6	0.77644 (13)	0.26899 (15)	0.20522 (11)	0.0290 (3)
O4	1.24853 (15)	0.84619 (15)	0.44292 (13)	0.0358 (4)
O5	0.84082 (15)	0.13655 (16)	0.07352 (13)	0.0369 (4)
N2	0.49854 (15)	0.19756 (15)	0.13786 (13)	0.0197 (3)
N1	0.78775 (14)	0.55439 (15)	0.65415 (12)	0.0170 (3)
O8	−0.01846 (14)	−0.02347 (15)	0.31525 (14)	0.0353 (3)
C1	0.51603 (18)	0.49910 (17)	0.72134 (16)	0.0197 (4)
C15	0.87163 (17)	0.55335 (17)	0.42150 (15)	0.0174 (3)
C7	0.77072 (18)	0.55219 (17)	0.77071 (15)	0.0184 (3)
C30	0.39099 (17)	0.21157 (17)	0.36530 (16)	0.0192 (3)
C10	1.07282 (18)	0.73894 (18)	0.54070 (16)	0.0210 (4)
H10	1.1224	0.7938	0.6141	0.025*
C23	0.37476 (18)	0.13821 (18)	0.14529 (16)	0.0211 (4)
H23	0.3153	0.0877	0.0750	0.025*
C2	0.64427 (18)	0.52756 (17)	0.80196 (15)	0.0191 (3)
C29	0.32105 (19)	0.19819 (19)	0.45757 (16)	0.0236 (4)
H29	0.3668	0.2427	0.5342	0.028*
C8	0.90317 (18)	0.63124 (18)	0.64082 (15)	0.0191 (3)
H8	0.9647	0.6868	0.7087	0.023*
C16	0.76517 (18)	0.19539 (19)	0.10052 (17)	0.0240 (4)
C22	0.53234 (18)	0.19068 (17)	0.02414 (15)	0.0208 (4)
C6	0.88014 (19)	0.5737 (2)	0.85524 (16)	0.0243 (4)
H6	0.9639	0.5880	0.8347	0.029*
C9	0.94566 (17)	0.63919 (18)	0.53175 (15)	0.0174 (3)
C24	0.31906 (18)	0.14162 (18)	0.24996 (16)	0.0202 (4)
C11	1.12378 (19)	0.75570 (19)	0.44233 (17)	0.0232 (4)
C26	0.11468 (18)	0.05233 (19)	0.32383 (18)	0.0246 (4)
C14	0.92307 (19)	0.5770 (2)	0.32232 (16)	0.0236 (4)
H14	0.8734	0.5249	0.2483	0.028*
C13	1.0464 (2)	0.6763 (2)	0.33279 (17)	0.0271 (4)
H13	1.0785	0.6905	0.2656	0.033*
C28	0.18627 (19)	0.12073 (19)	0.43753 (17)	0.0259 (4)
H28	0.1426	0.1140	0.5005	0.031*

C17	0.65857 (18)	0.18987 (18)	0.00625 (16)	0.0216 (4)
C3	0.6339 (2)	0.5301 (2)	0.91729 (17)	0.0281 (4)
H3	0.5506	0.5163	0.9388	0.034*
C18	0.6888 (2)	0.1836 (2)	−0.10535 (17)	0.0283 (4)
H18	0.7713	0.1803	−0.1186	0.034*
C21	0.4427 (2)	0.1897 (2)	−0.06769 (17)	0.0271 (4)
H21	0.3595	0.1919	−0.0555	0.032*
C19	0.5997 (2)	0.1820 (2)	−0.19642 (18)	0.0338 (5)
H19	0.6223	0.1786	−0.2699	0.041*
C5	0.8660 (2)	0.5741 (2)	0.96909 (17)	0.0297 (4)
H5	0.9400	0.5890	1.0243	0.036*
C25	0.17955 (18)	0.06293 (19)	0.23137 (17)	0.0241 (4)
H25	0.1318	0.0181	0.1554	0.029*
C20	0.4764 (2)	0.1855 (2)	−0.17737 (18)	0.0325 (5)
H20	0.4159	0.1851	−0.2382	0.039*
C4	0.7419 (2)	0.5523 (2)	1.00098 (17)	0.0324 (5)
H4	0.7317	0.5527	1.0774	0.039*
C12	1.3242 (2)	0.9314 (2)	0.55455 (19)	0.0342 (5)
H12A	1.4053	0.9963	0.5449	0.051*
H12B	1.3463	0.8783	0.6003	0.051*
H12C	1.2723	0.9773	0.5939	0.051*
C27	−0.0917 (2)	−0.1014 (3)	0.2011 (2)	0.0463 (6)
H27A	−0.1006	−0.0426	0.1558	0.069*
H27B	−0.1792	−0.1592	0.2063	0.069*
H27C	−0.0450	−0.1551	0.1640	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01381 (11)	0.02307 (12)	0.01270 (11)	0.00514 (9)	0.00312 (8)	0.00024 (8)
Cu2	0.01423 (11)	0.02633 (12)	0.01317 (11)	0.00607 (9)	0.00153 (8)	−0.00229 (9)
O7	0.0166 (6)	0.0229 (6)	0.0155 (6)	0.0037 (5)	0.0029 (5)	0.0009 (5)
O3	0.0139 (6)	0.0260 (6)	0.0134 (6)	0.0045 (5)	0.0025 (5)	0.0001 (5)
O2	0.0180 (6)	0.0296 (7)	0.0161 (6)	0.0071 (5)	0.0052 (5)	0.0003 (5)
O1	0.0226 (7)	0.0365 (8)	0.0217 (7)	0.0141 (6)	0.0114 (5)	0.0092 (6)
O6	0.0197 (7)	0.0425 (8)	0.0194 (7)	0.0144 (6)	0.0016 (5)	−0.0042 (6)
O4	0.0296 (8)	0.0351 (8)	0.0319 (8)	−0.0017 (6)	0.0149 (6)	0.0067 (6)
O5	0.0294 (8)	0.0448 (9)	0.0349 (8)	0.0219 (7)	0.0051 (6)	−0.0033 (7)
N2	0.0190 (7)	0.0212 (7)	0.0149 (7)	0.0063 (6)	0.0028 (6)	−0.0002 (6)
N1	0.0149 (7)	0.0222 (7)	0.0131 (7)	0.0066 (6)	0.0038 (5)	0.0034 (6)
O8	0.0180 (7)	0.0395 (8)	0.0386 (9)	0.0010 (6)	0.0072 (6)	0.0067 (7)
C1	0.0202 (9)	0.0187 (8)	0.0200 (9)	0.0060 (7)	0.0072 (7)	0.0059 (7)
C15	0.0157 (8)	0.0216 (8)	0.0175 (8)	0.0106 (7)	0.0032 (6)	0.0047 (7)
C7	0.0219 (9)	0.0200 (8)	0.0126 (8)	0.0074 (7)	0.0049 (7)	0.0036 (7)
C30	0.0178 (8)	0.0172 (8)	0.0216 (9)	0.0062 (7)	0.0035 (7)	0.0042 (7)
C10	0.0187 (9)	0.0214 (9)	0.0201 (9)	0.0058 (7)	0.0043 (7)	0.0031 (7)
C23	0.0189 (9)	0.0208 (9)	0.0179 (8)	0.0056 (7)	0.0000 (7)	−0.0007 (7)
C2	0.0218 (9)	0.0190 (8)	0.0165 (8)	0.0077 (7)	0.0065 (7)	0.0040 (7)

C29	0.0255 (10)	0.0226 (9)	0.0192 (9)	0.0052 (8)	0.0051 (7)	0.0048 (7)
C8	0.0176 (8)	0.0226 (9)	0.0140 (8)	0.0061 (7)	0.0013 (7)	0.0025 (7)
C16	0.0183 (9)	0.0251 (9)	0.0230 (9)	0.0055 (7)	0.0058 (7)	−0.0001 (7)
C22	0.0206 (9)	0.0181 (8)	0.0157 (9)	0.0029 (7)	0.0024 (7)	−0.0031 (7)
C6	0.0212 (9)	0.0324 (10)	0.0181 (9)	0.0099 (8)	0.0044 (7)	0.0052 (8)
C9	0.0161 (8)	0.0218 (8)	0.0162 (8)	0.0093 (7)	0.0043 (6)	0.0053 (7)
C24	0.0176 (9)	0.0197 (8)	0.0210 (9)	0.0059 (7)	0.0037 (7)	0.0035 (7)
C11	0.0216 (9)	0.0228 (9)	0.0261 (10)	0.0073 (7)	0.0098 (8)	0.0083 (8)
C26	0.0178 (9)	0.0227 (9)	0.0314 (10)	0.0057 (7)	0.0056 (8)	0.0069 (8)
C14	0.0253 (10)	0.0307 (10)	0.0143 (9)	0.0107 (8)	0.0048 (7)	0.0045 (7)
C13	0.0328 (11)	0.0316 (10)	0.0207 (10)	0.0122 (9)	0.0127 (8)	0.0110 (8)
C28	0.0248 (10)	0.0251 (9)	0.0274 (10)	0.0068 (8)	0.0105 (8)	0.0085 (8)
C17	0.0224 (9)	0.0174 (8)	0.0195 (9)	0.0053 (7)	0.0044 (7)	−0.0016 (7)
C3	0.0291 (10)	0.0374 (11)	0.0221 (10)	0.0130 (9)	0.0128 (8)	0.0123 (8)
C18	0.0281 (10)	0.0267 (10)	0.0251 (10)	0.0077 (8)	0.0103 (8)	−0.0001 (8)
C21	0.0230 (10)	0.0304 (10)	0.0217 (10)	0.0070 (8)	0.0018 (8)	0.0017 (8)
C19	0.0416 (12)	0.0362 (11)	0.0183 (10)	0.0096 (10)	0.0117 (9)	0.0030 (8)
C5	0.0322 (11)	0.0394 (12)	0.0171 (9)	0.0145 (9)	0.0007 (8)	0.0072 (8)
C25	0.0185 (9)	0.0235 (9)	0.0248 (10)	0.0052 (7)	0.0010 (7)	0.0019 (7)
C20	0.0346 (11)	0.0380 (12)	0.0184 (10)	0.0088 (9)	0.0008 (8)	0.0044 (8)
C4	0.0405 (12)	0.0456 (12)	0.0158 (9)	0.0183 (10)	0.0097 (8)	0.0121 (9)
C12	0.0241 (10)	0.0318 (11)	0.0386 (12)	0.0005 (9)	0.0065 (9)	0.0102 (9)
C27	0.0199 (11)	0.0551 (15)	0.0461 (14)	−0.0022 (10)	0.0002 (10)	0.0085 (12)

Geometric parameters (Å, º)

Cu1—Cu2	3.0091 (3)	C29—H29	0.9300
Cu1—O7	2.0122 (12)	C29—C28	1.377 (3)
Cu1—O3	1.8991 (12)	C8—H8	0.9300
Cu1—O2	1.8810 (12)	C8—C9	1.435 (2)
Cu1—N1	1.9530 (14)	C16—C17	1.510 (3)
Cu2—O7	1.9692 (12)	C22—C17	1.401 (3)
Cu2—O3	1.9552 (12)	C22—C21	1.391 (3)
Cu2—O1^{i}	2.3276 (14)	C6—H6	0.9300
Cu2—O6	1.9117 (13)	C6—C5	1.384 (3)
Cu2—N2	1.9295 (15)	C24—C25	1.424 (3)
O7—C30	1.345 (2)	C11—C13	1.393 (3)
O3—C15	1.343 (2)	C26—C28	1.394 (3)
O2—C1	1.288 (2)	C26—C25	1.370 (3)
O1—Cu2^{i}	2.3276 (14)	C14—H14	0.9300
O1—C1	1.238 (2)	C14—C13	1.378 (3)
O6—C16	1.291 (2)	C13—H13	0.9300
O4—C11	1.375 (2)	C28—H28	0.9300
O4—C12	1.421 (3)	C17—C18	1.396 (3)
O5—C16	1.226 (2)	C3—H3	0.9300
N2—C23	1.295 (2)	C3—C4	1.377 (3)
N2—C22	1.433 (2)	C18—H18	0.9300
N1—C7	1.429 (2)	C18—C19	1.378 (3)

N1—C8	1.295 (2)	C21—H21	0.9300
O8—C26	1.375 (2)	C21—C20	1.389 (3)
O8—C27	1.419 (3)	C19—H19	0.9300
C1—C2	1.503 (3)	C19—C20	1.383 (3)
C15—C9	1.406 (2)	C5—H5	0.9300
C15—C14	1.398 (2)	C5—C4	1.385 (3)
C7—C2	1.403 (2)	C25—H25	0.9300
C7—C6	1.396 (3)	C20—H20	0.9300
C30—C29	1.403 (3)	C4—H4	0.9300
C30—C24	1.412 (3)	C12—H12A	0.9600
C10—H10	0.9300	C12—H12B	0.9600
C10—C9	1.412 (2)	C12—H12C	0.9600
C10—C11	1.370 (3)	C27—H27A	0.9600
C23—H23	0.9300	C27—H27B	0.9600
C23—C24	1.437 (3)	C27—H27C	0.9600
C2—C3	1.390 (3)		

O7—Cu1—Cu2	40.37 (3)	O6—C16—C17	117.57 (16)
O3—Cu1—Cu2	39.35 (4)	O5—C16—O6	123.24 (18)
O3—Cu1—O7	79.07 (5)	O5—C16—C17	119.07 (17)
O3—Cu1—N1	93.19 (6)	C17—C22—N2	119.80 (16)
O2—Cu1—Cu2	134.83 (4)	C21—C22—N2	120.50 (17)
O2—Cu1—O7	98.20 (5)	C21—C22—C17	119.66 (17)
O2—Cu1—O3	166.96 (6)	C7—C6—H6	119.5
O2—Cu1—N1	93.64 (6)	C5—C6—C7	121.07 (18)
N1—Cu1—Cu2	131.52 (4)	C5—C6—H6	119.5
N1—Cu1—O7	158.21 (6)	C15—C9—C10	120.11 (16)
O7—Cu2—Cu1	41.44 (4)	C15—C9—C8	124.40 (16)
O7—Cu2—O1^{i}	93.92 (5)	C10—C9—C8	115.47 (16)
O3—Cu2—Cu1	38.01 (4)	C30—C24—C23	125.75 (16)
O3—Cu2—O7	78.81 (5)	C30—C24—C25	119.47 (17)
O3—Cu2—O1^{i}	85.67 (5)	C25—C24—C23	114.76 (16)
O1^{i}—Cu2—Cu1	84.04 (3)	O4—C11—C13	116.30 (16)
O6—Cu2—Cu1	128.39 (4)	C10—C11—O4	124.59 (17)
O6—Cu2—O7	143.58 (6)	C10—C11—C13	119.10 (17)
O6—Cu2—O3	95.61 (5)	O8—C26—C28	115.25 (17)
O6—Cu2—O1^{i}	121.77 (6)	C25—C26—O8	125.38 (18)
O6—Cu2—N2	94.18 (6)	C25—C26—C28	119.37 (17)
N2—Cu2—Cu1	134.27 (4)	C15—C14—H14	119.5
N2—Cu2—O7	95.11 (6)	C13—C14—C15	120.90 (17)
N2—Cu2—O3	169.71 (6)	C13—C14—H14	119.5
N2—Cu2—O1^{i}	86.48 (6)	C11—C13—H13	119.5
Cu2—O7—Cu1	98.18 (5)	C14—C13—C11	121.08 (17)
C30—O7—Cu1	132.32 (11)	C14—C13—H13	119.5
C30—O7—Cu2	125.98 (11)	C29—C28—C26	120.69 (18)
Cu1—O3—Cu2	102.64 (6)	C29—C28—H28	119.7
C15—O3—Cu1	124.31 (11)	C26—C28—H28	119.7
C15—O3—Cu2	129.03 (11)	C22—C17—C16	124.12 (16)

C1—O2—Cu1	129.79 (12)	C18—C17—C16	117.36 (17)
C1—O1—Cu2^{i}	113.00 (12)	C18—C17—C22	118.52 (18)
C16—O6—Cu2	126.44 (12)	C2—C3—H3	118.7
C11—O4—C12	116.00 (15)	C4—C3—C2	122.61 (19)
C23—N2—Cu2	123.84 (13)	C4—C3—H3	118.7
C23—N2—C22	118.75 (15)	C17—C18—H18	119.1
C22—N2—Cu2	116.89 (11)	C19—C18—C17	121.76 (19)
C7—N1—Cu1	120.52 (11)	C19—C18—H18	119.1
C8—N1—Cu1	122.04 (12)	C22—C21—H21	119.7
C8—N1—C7	117.43 (15)	C20—C21—C22	120.51 (19)
C26—O8—C27	116.52 (16)	C20—C21—H21	119.7
O2—C1—C2	120.14 (15)	C18—C19—H19	120.3
O1—C1—O2	121.74 (17)	C18—C19—C20	119.31 (19)
O1—C1—C2	118.12 (16)	C20—C19—H19	120.3
O3—C15—C9	121.09 (15)	C6—C5—H5	119.9
O3—C15—C14	120.93 (16)	C6—C5—C4	120.21 (19)
C14—C15—C9	117.97 (16)	C4—C5—H5	119.9
C2—C7—N1	120.78 (16)	C24—C25—H25	119.5
C6—C7—N1	120.26 (16)	C26—C25—C24	120.96 (18)
C6—C7—C2	118.96 (16)	C26—C25—H25	119.5
O7—C30—C29	120.21 (16)	C21—C20—H20	119.9
O7—C30—C24	121.92 (16)	C19—C20—C21	120.2 (2)
C29—C30—C24	117.86 (16)	C19—C20—H20	119.9
C9—C10—H10	119.7	C3—C4—C5	118.65 (18)
C11—C10—H10	119.7	C3—C4—H4	120.7
C11—C10—C9	120.61 (17)	C5—C4—H4	120.7
N2—C23—H23	116.4	O4—C12—H12A	109.5
N2—C23—C24	127.25 (16)	O4—C12—H12B	109.5
C24—C23—H23	116.4	O4—C12—H12C	109.5
C7—C2—C1	125.76 (16)	H12A—C12—H12B	109.5
C3—C2—C1	115.76 (16)	H12A—C12—H12C	109.5
C3—C2—C7	118.47 (17)	H12B—C12—H12C	109.5
C30—C29—H29	119.2	O8—C27—H27A	109.5
C28—C29—C30	121.65 (18)	O8—C27—H27B	109.5
C28—C29—H29	119.2	O8—C27—H27C	109.5
N1—C8—H8	116.7	H27A—C27—H27B	109.5
N1—C8—C9	126.52 (16)	H27A—C27—H27C	109.5
C9—C8—H8	116.7	H27B—C27—H27C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O6	0.93	2.55	3.112 (3)	119
C29—H29···O2	0.93	2.28	2.945 (2)	128

C23—H23···O5^{ii}	0.93	2.58	3.432 (2)	153
C27—H27*A*···O5^{iii}	0.96	2.63	3.567 (3)	165

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