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Crystal structure of a heterometallic coordination polymer: poly[diaquabis(μ_7-benzene-1,3,5-tricarboxylato)dicalcium(II)copper(II)]

Feng Zhang* and Bing-Guang Zhang

Key Laboratory of Catalysis and Materials Sciences of the State Ethnic Affairs Commission & Ministry of Education, College of Chemistry and Material Science, South-Central University for Nationalities, Wuhan 430074, People's Republic of China. *Correspondence e-mail: zhangbg68@yahoo.com

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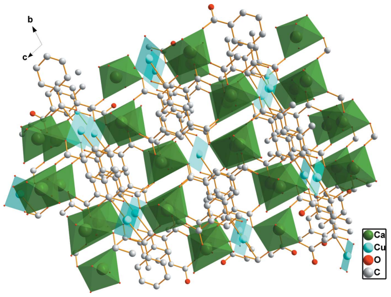
In the title complex, $[Ca_2Cu(C_9H_3O_6)_2(H_2O)_2]_n$, the Ca^{II} and Cu^{II} cations are bridged by the benzene-1,3,5-tricarboxylate anions (BTC^{3-}) to form the coordination polymer, in which each BTC^{3-} anion bridges two Cu^{II} and five Ca^{II} cations with a μ_7 coordination mode. The Cu^{II} cation, located at an inversion centre, is in a nearly square-planar geometry defined by four O atoms from four bridging BTC^{3-} anions, while the Ca^{II} cation is in a distorted octahedral geometry defined by five O atoms from bridging BTC^{3-} anions and one water molecule. O—H$\cdots$O hydrogen bonds between coordinating water molecules and carboxyl groups further stabilize the structure; π–π stacking is also observed between parallel benzene rings, the centroid-to-centroid distance being 3.357 (2) Å.



1. Chemical context

In recent years, the rational design and synthesis of heterometallic coordination compounds have attracted much attention due to their potential applications in magnetism, luminescence, adsorption, chemical sensing and catalysis, as well as their aesthetically beautiful architectures and topologies (Cui *et al.*, 2012; Huang *et al.*, 2013; Ma *et al.*, 2014; Wimberg *et al.*, 2012). However, hererometallic organic frameworks are investigated less frequently than single-metal organic frameworks in crystal engineering, mainly because of the competitive complexation of different metal ions in the self-assembly progress. Recently, alkaline-earth metal ions have attracted more and more research interest owing to their unpredictable coordination number and pH-dependent self-assembly in the construction of novel topological coordination compounds (Borah *et al.*, 2011; Chen *et al.*, 2011). However, the larger atomic radii and high enthalpy of hydration make it relatively difficult to design the coordination polymers of alkaline-earth metal ions as well as to synthesize them from aqueous solution (Reger *et al.*, 2013). As alkaline-earth metals and transition metals coordinate to the same ligand, it often gives rise to homometallic coordination compounds rather than heterometallic ones. In this regard, one of the effective synthetic strategies in building the alkaline-earth-metal-containing compounds is to employ appropriate bridging ligands. As a multifunctional hybrid ligand, H_3BTC (benzene-1,3,5-tricarboxylic acid) in its partly or fully deprotonated form exhibits versatile coordination modes and can bind to the metal ions by making full use of the carboxylate oxygen atoms. In addition, heterometallic compounds incorporating only the

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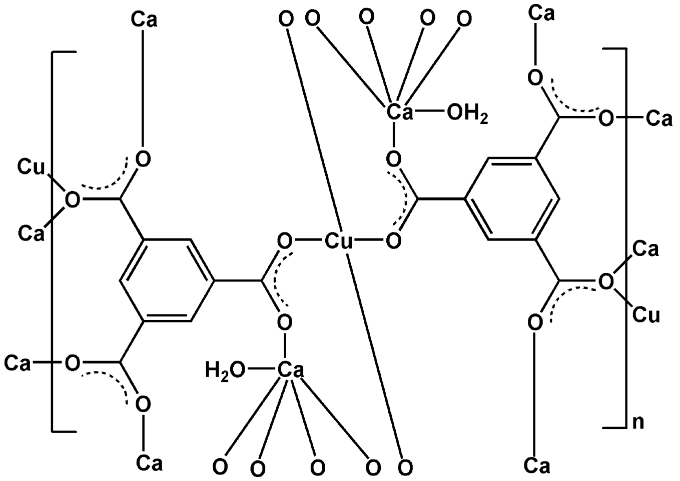
H_3BTC ligand are few in number (Chen *et al.*, 2004; Li *et al.*, 2010; Sun *et al.*, 2014, 2016; Xu *et al.*, 2014). As part of our ongoing studies on these compounds, we describe here synthesis and crystal structure of the title compound, $[Ca_2Cu(BTC)_2(H_2O)_2]_n$, (**1**).



2. Structural commentary

The asymmetric unit of (**1**) contains one copper(II) cation (located at an inversion centre), one calcium(II) cation, one BTC^{3-} anion and one coordinating water molecule (Fig. 1). The Cu—O bond lengths are in the range 1.9435 (19)–1.9800 (19) Å and the Ca—O bond lengths are in the range of 2.280 (2)–2.466 (2) Å (Table 1). All data are comparable to those reported for other related Cu^{II}–BTC and Ca^{II}–BTC complexes (Chui *et al.*, 1999; Yang *et al.*, 2004) . Each Cu^{II} cation is four-coordinated by four oxygen atoms from four different BTC^{3-} anions, forming a nearly square-planar geometry. Each Ca^{II} cation is six-coordinated by five carboxylate oxygen atoms from five different BTC^{3-} anions and one terminal water molecule, displaying a distorted octahedron (Fig. 1). The mean deviation of the equatorial plane constructed by atoms O1, O4, O6 and O*W*1 is 0.06 Å. The H_3BTC molecule is fully deprotonated and bridges two Cu^{II} ions and five Ca^{II} ions in a μ_7 coordination mode.

Table 1
Selected bond lengths (Å).

Ca1—O1	2.338 (2)	Ca1—O6^{iv}	2.357 (2)
Ca1—O3^{i}	2.280 (2)	Ca1—O*W*1	2.390 (2)
Ca1—O4^{ii}	2.333 (2)	Cu1—O2	1.9435 (19)
Ca1—O5^{iii}	2.466 (2)	Cu1—O5^{v}	1.9800 (19)

Symmetry codes: (i) $x, y, z-1$; (ii) $-x, -y+1, -z+2$; (iii) $x, y+1, z$; (iv) $-x, -y+1, -z+1$; (v) $-x+1, -y+1, -z+2$.

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O*W*1—H*W*1*A*···O4^{v}	0.84 (1)	1.95 (1)	2.793 (3)	173 (3)
O*W*1—H*W*1*B*···O2^{vi}	0.84 (1)	2.31 (2)	3.020 (3)	143 (3)

Symmetry codes: (v) $-x+1, -y+1, -z+2$; (vi) $-x+1, -y+2, -z+2$.

3. Supramolecular features

Each CuO_4 quadrilateral shares a vertex (O5) with two CaO_6 polyhedra to form a trinuclear unit $\{CuCa_2O_{14}\}$ with Ca–O–Cu–O–Ca connectivity (Fig. 2). Such units are cross-linked by the μ_7-BTC^{3-} anions to create a three-dimensional framework (Fig. 3). In addition, the terminal water molecule is hydrogen bonded to the carboxylate O atoms (Table 2), forming a two-dimensional network parallel to (100). π-π stacking interactions between (C1–C6) benzene rings $[Cg\cdots Cg(-x, 1-y, 2-z) = 3.357\ (2)$ Å$]$ further stabilize the crystal structure.

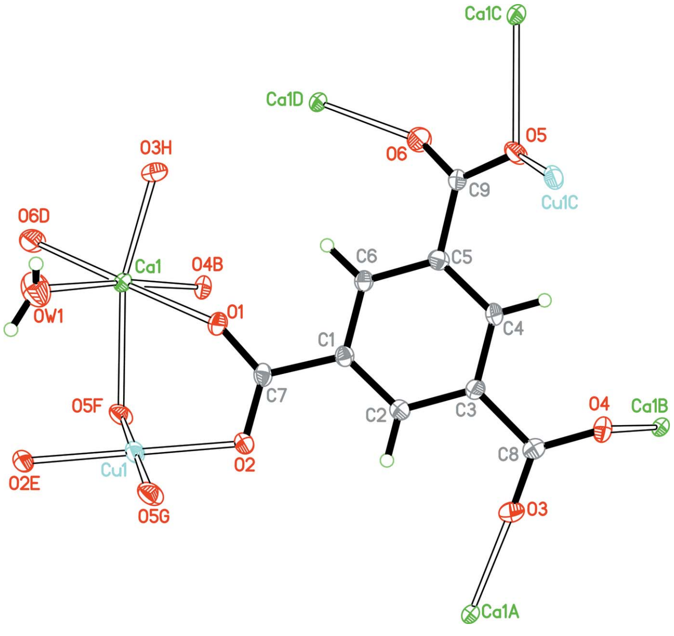


Figure 1
The coordination mode and atom-numbering scheme for (**1**). Displacement ellipsoids for non H-atoms are drawn at the 50% probability level, with H atoms shown as spheres of arbitrary radius. [Symmetry codes: (*A*) $x, y, z+1$; (*B*) $-x, -y+1, -z+2$; (*C*) $x, y-1, z$; (*D*) $-x, -y+1, -z+1$; (*E*) $-x+1, -y+2, -z+2$; (*F*) $x, y+1, z$; (*G*) $-x+1, -y+1, -z+2$; (*H*) $x, y, z-1$.]

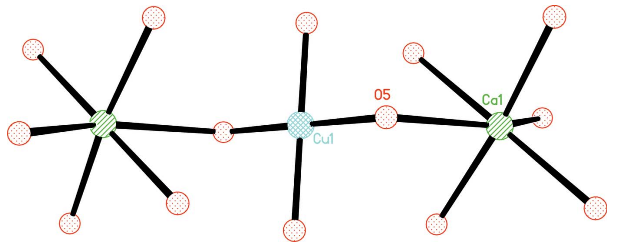


Figure 2
The trinuclear unit constructed from a $[CaO_6]$ octahedron and a $[CuO_4]$ quadrilateral.

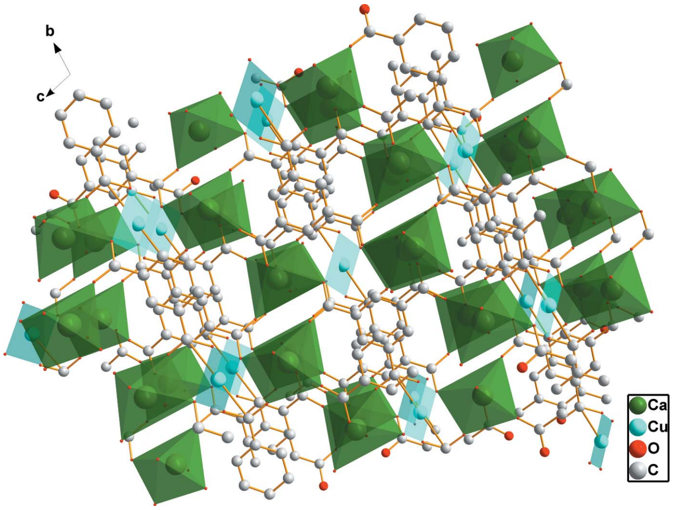


Figure 3
Polyhedral view of the three-dimensional heterometallic coordination framework of (**1**). All H atoms have been omitted for clarity.

4. Synthesis and crystallization

The title compound was synthesized using a similar procedure to that for the synthesis of the analogous compound $[CuSr_2(BTC)_2]\cdot 10H_2O$ (Sun *et al.*, 2016). A mixture of H_3BTC (210 mg, 1 mmol), $CuCl_2\cdot 6H_2O$ (121 mg, 0.5 mmol) and $CaCl_2$ (110 mg, 1 mmol) in 15 mL of distilled water was stirred for 10 min in air; 0.5 *M* NaOH was then added dropwise, and then the mixture was turned into a Parr Teflon-lined stainless steel vessel and heated to 443 K for 3 d. Blue block-shaped crystals suitable for X-ray diffraction were obtained in 60% yield (based on benzene-1,3,5-tricarboxylic acid).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms of the coordinating water molecule were located from a difference-Fourier map, but refined using a riding model with isotropic displacement parameters $U_{iso}(H) = 1.2U_{eq}(O)$. Hydrogen atoms attached to carbon atoms were positioned geometrically (C—H = 0.93 Å) and refined with $U_{iso}(H) = 1.2U_{eq}(C)$.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ca_2Cu(C_9H_3O_6)_2(H_2O)_2]$
M_r	593.96
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	6.664 (3), 8.754 (4), 8.925 (4)
α, β, γ (°)	103.065 (4), 110.140 (4), 92.776 (5)
V ($Å^3$)	471.6 (4)
Z	1
Radiation type	Mo *Kα*
μ (mm^{-1})	1.79
Crystal size (mm)	0.18 × 0.15 × 0.14
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.721, 0.766
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2442, 1635, 1588
R_{int}	0.012
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.029, 0.084, 1.04
No. of reflections	1635
No. of parameters	166
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.35, −0.68

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 2006).

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Crystal structure of a heterometallic coordination polymer: poly[diaquabis(μ_7-benzene-1,3,5-tricarboxylato)dicalcium(II)copper(II)]

Feng Zhang and Bing-Guang Zhang

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL97* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Poly[diaquabis(μ_7-benzene-1,3,5-tricarboxylato)dicalcium(II)copper(II)]

Crystal data

$[Ca_2Cu(C_9H_3O_6)_2(H_2O)_2]$
$M_r = 593.96$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.664$ (3) Å
$b = 8.754$ (4) Å
$c = 8.925$ (4) Å
$\alpha = 103.065$ (4)°
$\beta = 110.140$ (4)°
$\gamma = 92.776$ (5)°
$V = 471.6$ (4) Å^3
$Z = 1$
$F(000) = 299$
$D_x = 2.091$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1990 reflections
$\theta = 2.4$–27.5°
$\mu = 1.79$ mm^{-1}
$T = 296$ K
Block, blue
0.18 × 0.15 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
$T_{\min} = 0.721$, $T_{\max} = 0.766$
2442 measured reflections
1635 independent reflections
1588 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.012$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 2.4°$
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 4$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.084$
$S = 1.04$
1635 reflections
166 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.6456P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.13337 (8)	0.79200 (6)	0.58531 (6)	0.01430 (16)
Cu1	0.5000	1.0000	1.0000	0.01590 (16)
O1	0.2949 (3)	0.6981 (2)	0.8180 (2)	0.0206 (4)
O2	0.3877 (3)	0.8375 (2)	1.0782 (2)	0.0192 (4)
O3	0.2155 (4)	0.5598 (2)	1.4590 (2)	0.0273 (5)
O4	0.1993 (3)	0.2977 (2)	1.4102 (2)	0.0190 (4)
O5	0.2085 (3)	0.0033 (2)	0.8405 (2)	0.0186 (4)
O6	0.0233 (4)	0.1170 (2)	0.6527 (2)	0.0283 (5)
C1	0.2707 (4)	0.5610 (3)	1.0114 (3)	0.0126 (5)
C2	0.2808 (4)	0.5623 (3)	1.1690 (3)	0.0145 (5)
H2A	0.3166	0.6577	1.2499	0.017*
C3	0.2377 (4)	0.4211 (3)	1.2074 (3)	0.0136 (5)
C4	0.1929 (4)	0.2786 (3)	1.0883 (3)	0.0142 (5)
H4A	0.1703	0.1841	1.1148	0.017*
C5	0.1815 (4)	0.2765 (3)	0.9288 (3)	0.0142 (5)
C6	0.2163 (4)	0.4182 (3)	0.8895 (3)	0.0136 (5)
H6A	0.2034	0.4176	0.7822	0.016*
C7	0.3178 (4)	0.7085 (3)	0.9639 (3)	0.0139 (5)
C8	0.2195 (4)	0.4278 (3)	1.3728 (3)	0.0154 (5)
C9	0.1339 (4)	0.1255 (3)	0.7989 (3)	0.0142 (5)
OW1	0.4854 (3)	0.8960 (3)	0.6111 (3)	0.0315 (5)
HW1A	0.587 (4)	0.844 (3)	0.604 (4)	0.038*
HW1B	0.544 (5)	0.9871 (18)	0.669 (4)	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0188 (3)	0.0142 (3)	0.0099 (3)	0.0011 (2)	0.0048 (2)	0.0040 (2)
Cu1	0.0204 (3)	0.0110 (2)	0.0147 (3)	0.00010 (17)	0.00383 (19)	0.00479 (18)
O1	0.0344 (11)	0.0158 (9)	0.0143 (9)	0.0058 (8)	0.0090 (8)	0.0084 (7)
O2	0.0282 (10)	0.0125 (9)	0.0145 (9)	−0.0024 (7)	0.0056 (8)	0.0035 (7)
O3	0.0480 (13)	0.0191 (10)	0.0181 (10)	0.0061 (9)	0.0181 (10)	0.0016 (8)

O4	0.0236 (10)	0.0189 (10)	0.0181 (9)	0.0014 (7)	0.0094 (8)	0.0092 (8)
O5	0.0228 (10)	0.0107 (9)	0.0180 (9)	0.0032 (7)	0.0027 (8)	0.0030 (7)
O6	0.0452 (13)	0.0206 (10)	0.0118 (10)	0.0027 (9)	0.0010 (9)	0.0051 (8)
C1	0.0118 (12)	0.0128 (12)	0.0131 (12)	0.0020 (9)	0.0033 (10)	0.0049 (10)
C2	0.0160 (12)	0.0128 (12)	0.0141 (12)	0.0015 (9)	0.0051 (10)	0.0032 (10)
C3	0.0148 (12)	0.0140 (12)	0.0124 (12)	0.0025 (9)	0.0049 (10)	0.0043 (10)
C4	0.0169 (12)	0.0119 (12)	0.0155 (12)	0.0035 (9)	0.0057 (10)	0.0065 (10)
C5	0.0143 (12)	0.0135 (12)	0.0131 (12)	0.0032 (10)	0.0030 (10)	0.0033 (10)
C6	0.0159 (12)	0.0130 (12)	0.0125 (12)	0.0044 (10)	0.0040 (10)	0.0057 (10)
C7	0.0145 (12)	0.0135 (12)	0.0167 (13)	0.0051 (9)	0.0063 (10)	0.0078 (10)
C8	0.0154 (12)	0.0174 (13)	0.0130 (12)	0.0024 (10)	0.0047 (10)	0.0036 (10)
C9	0.0177 (12)	0.0129 (12)	0.0129 (13)	0.0017 (10)	0.0056 (10)	0.0050 (10)
OW1	0.0262 (11)	0.0264 (11)	0.0459 (14)	0.0047 (9)	0.0166 (10)	0.0116 (10)

Geometric parameters (Å, º)

Ca1—O1	2.338 (2)	O5—Ca1^{viii}	2.466 (2)
Ca1—O3^{i}	2.280 (2)	O6—C9	1.241 (3)
Ca1—O4^{ii}	2.333 (2)	O6—Ca1^{iv}	2.357 (2)
Ca1—O5^{iii}	2.466 (2)	O6—Ca1^{viii}	2.954 (2)
Ca1—O6^{iv}	2.357 (2)	C1—C2	1.382 (4)
Ca1—OW1	2.390 (2)	C1—C6	1.395 (4)
Ca1—Cu1	3.6439 (13)	C1—C7	1.499 (3)
Cu1—O2^{v}	1.9435 (19)	C2—C3	1.398 (4)
Cu1—O2	1.9435 (19)	C2—H2A	0.9300
Cu1—O5^{vi}	1.9800 (19)	C3—C4	1.386 (4)
Cu1—O5^{iii}	1.9800 (19)	C3—C8	1.511 (3)
Cu1—Ca1^{v}	3.6439 (13)	C4—C5	1.395 (4)
O1—C7	1.239 (3)	C4—H4A	0.9300
O2—C7	1.278 (3)	C5—C6	1.393 (4)
O3—C8	1.242 (3)	C5—C9	1.485 (3)
O3—Ca1^{vii}	2.280 (2)	C6—H6A	0.9300
O4—C8	1.271 (3)	C8—Ca1^{ii}	3.141 (3)
O4—Ca1^{ii}	2.333 (2)	C9—Ca1^{viii}	3.104 (3)
O5—C9	1.278 (3)	OW1—HW1A	0.844 (10)
O5—Cu1^{viii}	1.9800 (19)	OW1—HW1B	0.836 (10)

O3^{i}—Ca1—O4^{ii}	99.86 (8)	C7—O2—Cu1	110.48 (16)
O3^{i}—Ca1—O1	81.17 (8)	C8—O3—Ca1^{vii}	168.1 (2)
O4^{ii}—Ca1—O1	87.46 (7)	C8—O4—Ca1^{ii}	118.28 (16)
O3^{i}—Ca1—O6^{iv}	97.47 (8)	C9—O5—Cu1^{viii}	125.84 (16)
O4^{ii}—Ca1—O6^{iv}	93.57 (8)	C9—O5—Ca1^{viii}	107.73 (15)
O1—Ca1—O6^{iv}	178.43 (7)	Cu1^{viii}—O5—Ca1^{viii}	109.61 (8)
O3^{i}—Ca1—OW1	83.82 (8)	C9—O6—Ca1^{iv}	157.26 (18)
O4^{ii}—Ca1—OW1	173.99 (8)	C9—O6—Ca1^{viii}	85.06 (15)
O1—Ca1—OW1	88.42 (8)	Ca1^{iv}—O6—Ca1^{viii}	114.30 (8)
O6^{iv}—Ca1—OW1	90.64 (8)	C2—C1—C6	120.0 (2)
O3^{i}—Ca1—O5^{iii}	148.03 (7)	C2—C1—C7	122.6 (2)

O4^{ii}—Ca1—O5^{iii}	91.33 (7)	C6—C1—C7	117.4 (2)
O1—Ca1—O5^{iii}	69.43 (7)	C1—C2—C3	120.3 (2)
O6^{iv}—Ca1—O5^{iii}	111.71 (7)	C1—C2—H2A	119.8
OW1—Ca1—O5^{iii}	83.12 (7)	C3—C2—H2A	119.8
O3^{i}—Ca1—Cu1	118.21 (6)	C4—C3—C2	119.6 (2)
O4^{ii}—Ca1—Cu1	110.50 (5)	C4—C3—C8	120.9 (2)
O1—Ca1—Cu1	49.46 (5)	C2—C3—C8	119.2 (2)
O6^{iv}—Ca1—Cu1	131.04 (6)	C3—C4—C5	120.3 (2)
OW1—Ca1—Cu1	63.49 (6)	C3—C4—H4A	119.9
O5^{iii}—Ca1—Cu1	30.79 (4)	C5—C4—H4A	119.9
O6^{iii}—Ca1—Cu1	73.03 (4)	C6—C5—C4	119.8 (2)
C9^{iii}—Ca1—Cu1	50.47 (5)	C6—C5—C9	118.8 (2)
C8^{ii}—Ca1—Cu1	106.72 (6)	C4—C5—C9	121.4 (2)
O2^{v}—Cu1—O2	180.000 (1)	C5—C6—C1	119.9 (2)
O2^{v}—Cu1—O5^{vi}	91.13 (8)	C5—C6—H6A	120.1
O2—Cu1—O5^{vi}	88.87 (8)	C1—C6—H6A	120.1
O2^{v}—Cu1—O5^{iii}	88.87 (8)	O1—C7—O2	123.6 (2)
O2—Cu1—O5^{iii}	91.13 (8)	O1—C7—C1	118.5 (2)
O5^{vi}—Cu1—O5^{iii}	180.000 (1)	O2—C7—C1	117.8 (2)
O2^{v}—Cu1—Ca1^{v}	87.31 (6)	O3—C8—O4	124.8 (2)
O2—Cu1—Ca1^{v}	92.69 (6)	O3—C8—C3	117.4 (2)
O5^{vi}—Cu1—Ca1^{v}	39.61 (5)	O4—C8—C3	117.7 (2)
O5^{iii}—Cu1—Ca1^{v}	140.39 (5)	O6—C9—O5	120.3 (2)
O2^{v}—Cu1—Ca1	92.69 (6)	O6—C9—C5	121.0 (2)
O2—Cu1—Ca1	87.31 (6)	O5—C9—C5	118.7 (2)
O5^{vi}—Cu1—Ca1	140.39 (5)	Ca1—OW1—HW1A	127 (2)
O5^{iii}—Cu1—Ca1	39.61 (5)	Ca1—OW1—HW1B	122 (2)
Ca1^{v}—Cu1—Ca1	180.0	HW1A—OW1—HW1B	105.9 (16)
C7—O1—Ca1	146.05 (17)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*1—H*W*1*A*···O4^{vi}	0.84 (1)	1.95 (1)	2.793 (3)	173 (3)
O*W*1—H*W*1*B*···O2^{v}	0.84 (1)	2.31 (2)	3.020 (3)	143 (3)

Symmetry codes: (v) −*x*+1, −*y*+2, −*z*+2; (vi) −*x*+1, −*y*+1, −*z*+2.