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Poly[[tetraaquabis(1*H*-imidazole-κN^3)-bis[2-(oxaloamino)benzoato(3–)]-dicopper(II)barium(II)] dihydrate]

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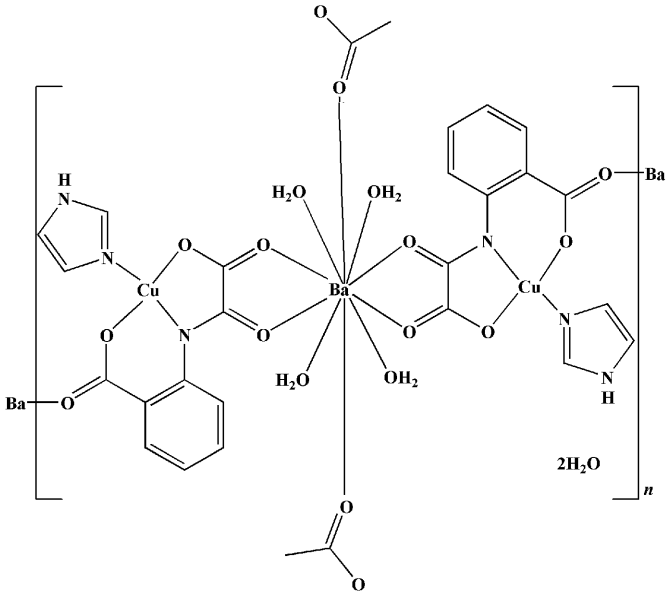
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; H-atom completeness 86%; disorder in solvent or counterion; R factor = 0.036; wR factor = 0.090; data-to-parameter ratio = 12.0.

In the title coordination polymer, $\{[BaCu_2(C_9H_4NO_5)_2(C_3H_4N_2)_2(H_2O)_4]\cdot 2H_2O\}_n$, the Ba^{2+} cation is decacoordinate, ligated by four aqua ligands and four $[Cu(C_9H_4O_5N)(C_3H_4N_2)]$ 'complex ligands'. The Cu^{II}-containing complex-ligands are bridged by the Ba^{2+} cations, resulting in a one-dimensional polymeric chain structure. The crystal structure is maintained *via* N—H···O and O—H···O hydrogen bonds. There is one disordered solvent water molecule in the asymmetric unit, with occupancies of 0.44 (2) and 0.56 (2).

Related literature

For related literature, see: Gao *et al.* (2001); Kahn (1993); Zang *et al.* (2003).



Experimental

Crystal data

$[BaCu_2(C_9H_4NO_5)_2(C_3H_4N_2)_2(H_2O)_4]\cdot 2H_2O$
M_r = 920.94
Monoclinic, $P2/c$
a = 10.662 (3) Å
b = 6.9165 (18) Å
c = 21.335 (5) Å
β = 101.146 (4)°
V = 1543.6 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.71 mm^{-1}
T = 293 (2) K
0.3 × 0.2 × 0.2 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.525, T_{max} = 0.583
7263 measured reflections
2713 independent reflections
2398 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.089
S = 1.01
2713 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.86	1.95	2.804 (5)	177
O5—H5B···O4^{ii}	0.85	1.99	2.827 (5)	169
O5—H5B···O8^{ii}	0.85	2.58	3.047 (5)	116
O9—H9A···O8^{iii}	0.95	2.08	2.915 (5)	145

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2076).

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Poly[[tetraaquabis(1*H*-imidazole-κN^3)bis[2-(oxaloamino)-benzoato(3–)]dicopper(II)barium(II)] dihydrate]

Chongzhen Mei, Kaihui Li and Peng Zhang

S1. Comment

Designing metal-containing building blocks to spontaneously assembly infinite molecular architectures is of considerable interest recently as a result of the peculiar magnetic exchange interactions between metal ions through bridging ligands (Kahn, 1993). Among many other methods, the "complex as ligand" approach, *i.e.* using metal cations to link reactively stable coordination compounds that contain potential bridging blocks, is particularly suitable for designing heteropolymetallic compounds, ranging from discrete entities to three-dimensional architectures. (Gao *et al.*, 2001)

In the title compound, Cu^{II} adopts a square planar geometry, coordinating to O3, O4 and N1 from the oxamato-N-benzoate and N2 from the imidazole ligand to afford a Cu-containing "ligand". Ba^{II}, lying on the 2-fold axis, is decacoordinate and bridges these Cu-ligands to form one-dimensional chains along the *c* axis.

S2. Experimental

0.232 g (1 mmol) oxamato-*N*-benzoic acid (Zang *et al.*, 2003) and 0.12 g (3 mmol) were dissolved in 20 ml water. To this solution, 0.17 g (1 mmol) $CuCl_2.2H_2O$ and 0.068 g (1 mmol) imidazole were added. After stirring for an hour, 0.208 g (1 mmol) $BaCl_2$ was added. The solution was filtered after stirring for another hour. Evaporation of the filtrate gave red single crystals of the title compound in one week.

S3. Refinement

The structure was solved by direct methods. All the H atoms were fixed geometrically and constrained with a riding model. d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic H atoms; 0.85 Å, $U_{iso} = 1.5U_{eq}$ (O) for H_2O hydrogen atoms.

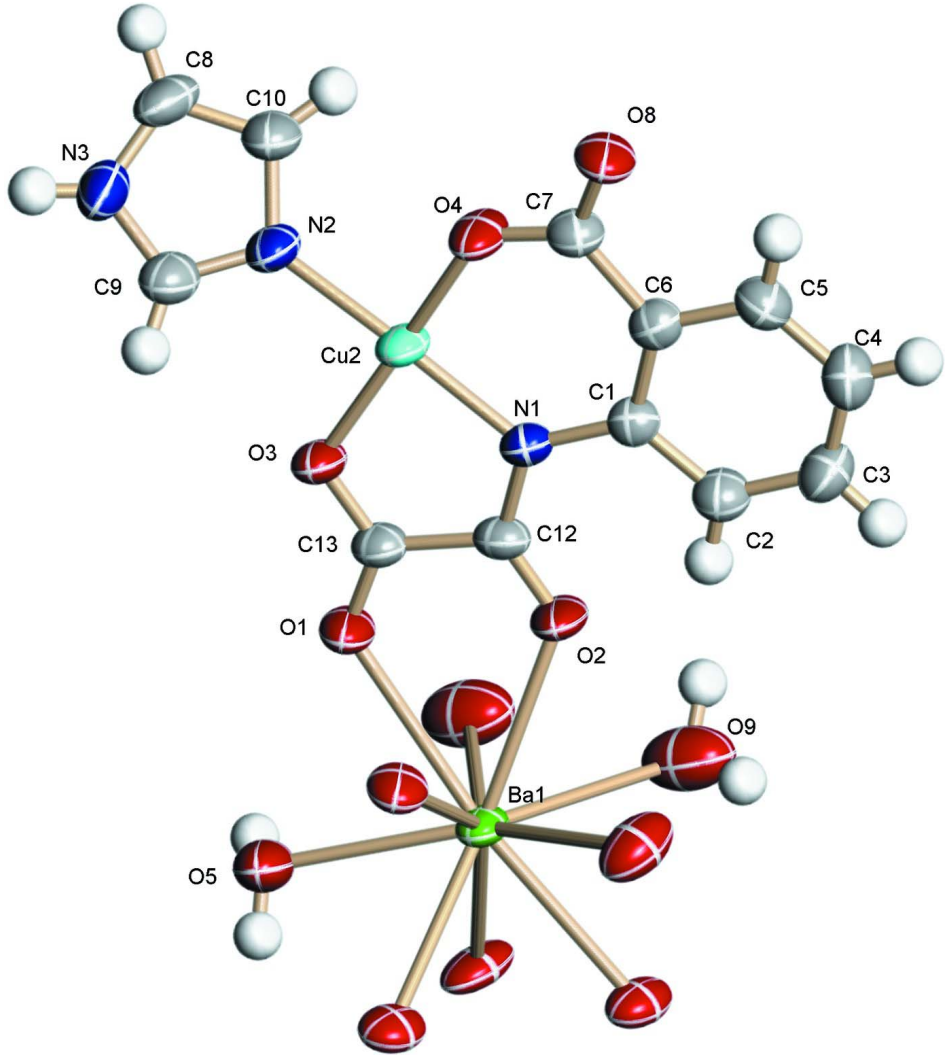

Figure 1

Asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. A disordered solvent water (O10) molecule has been omitted for clarity. Symmetry-equivalent O atoms generated about the Ba1 atom are at (1 - *x*, *y*, 1.5 - *z*), (1 - *x*, 2 - *y*, 2 - *z*) and (*x*, 2 - *y*, *z* - 1/2).

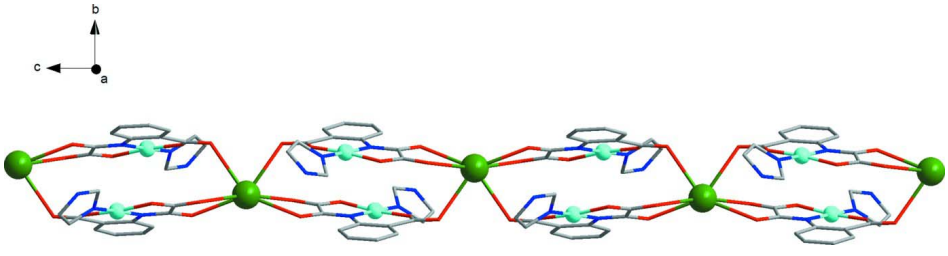

Figure 2

The one-dimensional polymeric chain viewed along the *c* axis. H atoms, aqueous ligands and solvent water molecules are omitted for clarity.

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Monoclinic, $P2/c$
Hall symbol: -P 2yc
$a = 10.662$ (3) Å
$b = 6.9165$ (18) Å
$c = 21.335$ (5) Å
$\beta = 101.146$ (4)°
$V = 1543.6$ (7) Å^3
$Z = 2$
$F(000) = 912$
$D_x = 1.981$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 857 reflections
$\theta = 3.0$–$27.3°$
$\mu = 2.71$ mm^{-1}
$T = 293$ K
Block, red
0.3 × 0.2 × 0.2 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.525$, $T_{max} = 0.583$
7263 measured reflections
2713 independent reflections
2398 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
$h = -12\rightarrow12$
$k = -8\rightarrow8$
$l = -25\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.089$
$S = 1.01$
2713 reflections
226 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
Ba1	0.5000	0.90568 (5)	0.7500	0.03268 (14)	
Cu2	0.70008 (4)	0.79877 (8)	1.03715 (2)	0.03358 (16)	
C1	0.4210 (4)	0.7210 (6)	0.9961 (2)	0.0308 (9)	
C2	0.3109 (4)	0.6829 (7)	0.9499 (2)	0.0413 (10)	

H2	0.3156	0.6890	0.9069	0.050*	
C3	0.1959 (4)	0.6366 (7)	0.9667 (2)	0.0459 (12)	
H3	0.1245	0.6136	0.9350	0.055*	
C4	0.1856 (4)	0.6243 (7)	1.0289 (2)	0.0460 (12)	
H4	0.1082	0.5917	1.0401	0.055*	
C5	0.2922 (4)	0.6609 (7)	1.0754 (2)	0.0415 (10)	
H5	0.2856	0.6533	1.1182	0.050*	
C6	0.4103 (4)	0.7096 (6)	1.0598 (2)	0.0334 (9)	
C7	0.5146 (4)	0.7449 (7)	1.1180 (2)	0.0362 (10)	
C8	1.0359 (4)	0.7848 (9)	1.1711 (2)	0.0550 (14)	
H8	1.0897	0.7403	1.2078	0.066*	
C9	0.9614 (4)	0.9421 (7)	1.0840 (2)	0.0464 (12)	
H9	0.9563	1.0274	1.0499	0.056*	
C10	0.9169 (4)	0.7209 (8)	1.1470 (2)	0.0479 (12)	
H10	0.8736	0.6250	1.1648	0.058*	
C12	0.5519 (4)	0.7837 (6)	0.91832 (19)	0.0345 (10)	
C13	0.6890 (4)	0.8380 (7)	0.91134 (19)	0.0339 (9)	
N1	0.5387 (3)	0.7682 (5)	0.97887 (15)	0.0301 (7)	
N2	0.8704 (3)	0.8215 (6)	1.09186 (17)	0.0390 (8)	
N3	1.0623 (3)	0.9254 (6)	1.13173 (18)	0.0484 (10)	
H3A	1.1315	0.9922	1.1365	0.058*	
O1	0.7097 (3)	0.8641 (5)	0.85734 (13)	0.0460 (8)	
O2	0.4736 (3)	0.7653 (6)	0.86823 (14)	0.0549 (10)	
O3	0.7724 (2)	0.8539 (5)	0.96263 (13)	0.0412 (7)	
O4	0.6293 (3)	0.7678 (5)	1.11137 (13)	0.0466 (8)	
O5	0.7323 (3)	1.0322 (6)	0.72527 (16)	0.0648 (10)	
H5B	0.7114	1.0964	0.6909	0.097*	
H5C	0.7768	0.9304	0.7246	0.097*	
O8	0.4863 (3)	0.7515 (5)	1.17116 (14)	0.0462 (8)	
O9	0.3581 (4)	0.5293 (6)	0.7463 (2)	0.0893 (13)	
H9C	0.2794	0.5576	0.7421	0.134*	
H9A	0.3773	0.4384	0.7804	0.134*	
O10	0.874 (3)	0.681 (4)	0.7671 (15)	0.143 (6)	0.44 (2)
O10′	0.8713 (19)	0.711 (3)	0.7229 (13)	0.143 (6)	0.56 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0323 (2)	0.0479 (2)	0.01666 (19)	0.000	0.00160 (13)	0.000
Cu2	0.0342 (3)	0.0463 (4)	0.0181 (3)	0.0002 (2)	−0.0003 (2)	−0.0013 (2)
C1	0.035 (2)	0.028 (2)	0.029 (2)	0.0008 (17)	0.0056 (17)	−0.0027 (18)
C2	0.044 (2)	0.048 (3)	0.032 (2)	−0.002 (2)	0.0073 (19)	−0.003 (2)
C3	0.037 (2)	0.054 (3)	0.044 (3)	−0.003 (2)	0.000 (2)	−0.006 (3)
C4	0.039 (2)	0.045 (3)	0.056 (3)	−0.006 (2)	0.013 (2)	−0.006 (2)
C5	0.045 (2)	0.044 (3)	0.037 (2)	−0.001 (2)	0.013 (2)	0.004 (2)
C6	0.037 (2)	0.028 (2)	0.034 (2)	0.0018 (17)	0.0045 (18)	−0.0012 (19)
C7	0.041 (2)	0.040 (3)	0.026 (2)	0.0017 (19)	0.0055 (18)	−0.001 (2)
C8	0.040 (2)	0.090 (4)	0.031 (2)	0.007 (3)	−0.004 (2)	0.005 (3)

C9	0.044 (2)	0.063 (3)	0.032 (2)	0.002 (2)	0.007 (2)	0.004 (2)
C10	0.048 (2)	0.066 (3)	0.029 (2)	−0.006 (2)	0.003 (2)	0.007 (2)
C12	0.043 (2)	0.036 (3)	0.023 (2)	0.0002 (19)	0.0032 (18)	0.0035 (19)
C13	0.040 (2)	0.038 (2)	0.022 (2)	−0.0004 (19)	0.0019 (17)	0.000 (2)
N1	0.0336 (16)	0.0324 (19)	0.0228 (17)	0.0026 (14)	0.0013 (13)	0.0009 (15)
N2	0.0354 (18)	0.054 (2)	0.0247 (18)	−0.0018 (17)	−0.0015 (15)	−0.0008 (18)
N3	0.0347 (18)	0.070 (3)	0.039 (2)	−0.0095 (19)	0.0035 (16)	−0.005 (2)
O1	0.0424 (16)	0.074 (2)	0.0213 (15)	−0.0110 (16)	0.0058 (13)	0.0047 (16)
O2	0.0451 (16)	0.095 (3)	0.0201 (16)	−0.0169 (18)	−0.0047 (14)	0.0107 (18)
O3	0.0361 (14)	0.063 (2)	0.0225 (14)	−0.0028 (14)	0.0000 (12)	0.0063 (16)
O4	0.0384 (16)	0.082 (3)	0.0182 (14)	−0.0026 (15)	0.0034 (12)	−0.0059 (16)
O5	0.0491 (18)	0.099 (3)	0.0427 (19)	−0.0122 (19)	−0.0002 (15)	0.023 (2)
O8	0.0517 (17)	0.068 (2)	0.0209 (16)	−0.0074 (16)	0.0120 (13)	−0.0011 (15)
O9	0.126 (3)	0.073 (3)	0.059 (3)	0.002 (3)	−0.008 (3)	0.003 (2)
O10	0.115 (5)	0.122 (8)	0.198 (18)	0.027 (5)	0.045 (14)	−0.028 (15)
O10′	0.115 (5)	0.122 (8)	0.198 (18)	0.027 (5)	0.045 (14)	−0.028 (15)

Geometric parameters (Å, º)

Ba1—O2^{i}	2.767 (3)	C5—H5	0.9300
Ba1—O2	2.767 (3)	C6—C7	1.518 (6)
Ba1—O5	2.772 (3)	C7—O8	1.230 (5)
Ba1—O5^{i}	2.772 (3)	C7—O4	1.268 (5)
Ba1—O1^{i}	2.889 (3)	C8—C10	1.347 (6)
Ba1—O1	2.889 (3)	C8—N3	1.349 (6)
Ba1—O8^{ii}	2.894 (3)	C8—H8	0.9300
Ba1—O8^{iii}	2.894 (3)	C9—N2	1.314 (6)
Ba1—O9	3.004 (5)	C9—N3	1.335 (6)
Ba1—O9^{i}	3.004 (4)	C9—H9	0.9300
Cu2—O4	1.894 (3)	C10—N2	1.375 (6)
Cu2—N1	1.930 (3)	C10—H10	0.9300
Cu2—O3	1.934 (3)	C12—O2	1.229 (5)
Cu2—N2	1.966 (3)	C12—N1	1.331 (5)
C1—C6	1.389 (6)	C12—C13	1.544 (5)
C1—C2	1.404 (6)	C13—O1	1.228 (5)
C1—N1	1.412 (5)	C13—O3	1.274 (5)
C2—C3	1.380 (6)	N3—H3A	0.8600
C2—H2	0.9300	O5—H5B	0.8502
C3—C4	1.355 (7)	O5—H5C	0.8500
C3—H3	0.9300	O8—Ba1^{ii}	2.894 (3)
C4—C5	1.379 (6)	O9—H9C	0.8498
C4—H4	0.9300	O9—H9A	0.9530
C5—C6	1.404 (5)		

O2^{i}—Ba1—O2	138.93 (16)	C6—C1—C2	117.4 (3)
O2^{i}—Ba1—O5	71.64 (10)	C6—C1—N1	120.9 (4)
O2—Ba1—O5	122.44 (9)	C2—C1—N1	121.7 (4)
O2^{i}—Ba1—O5^{i}	122.44 (9)	C3—C2—C1	121.7 (4)

O2—Ba1—O5^{i}	71.64 (10)	C3—C2—H2	119.1
O5—Ba1—O5^{i}	143.21 (18)	C1—C2—H2	119.1
O2^{i}—Ba1—O1^{i}	56.10 (8)	C4—C3—C2	120.9 (4)
O2—Ba1—O1^{i}	119.20 (9)	C4—C3—H3	119.6
O5—Ba1—O1^{i}	117.63 (9)	C2—C3—H3	119.6
O5^{i}—Ba1—O1^{i}	66.37 (9)	C3—C4—C5	118.7 (4)
O2^{i}—Ba1—O1	119.20 (9)	C3—C4—H4	120.6
O2—Ba1—O1	56.10 (8)	C5—C4—H4	120.6
O5—Ba1—O1	66.37 (9)	C4—C5—C6	121.7 (4)
O5^{i}—Ba1—O1	117.63 (9)	C4—C5—H5	119.1
O1^{i}—Ba1—O1	168.57 (15)	C6—C5—H5	119.1
O2^{i}—Ba1—O8^{ii}	144.53 (10)	C1—C6—C5	119.5 (4)
O2—Ba1—O8^{ii}	76.13 (10)	C1—C6—C7	127.3 (3)
O5—Ba1—O8^{ii}	84.57 (10)	C5—C6—C7	113.2 (4)
O5^{i}—Ba1—O8^{ii}	65.01 (10)	O8—C7—O4	120.8 (4)
O1^{i}—Ba1—O8^{ii}	119.12 (9)	O8—C7—C6	119.3 (3)
O1—Ba1—O8^{ii}	71.12 (10)	O4—C7—C6	119.9 (3)
O2^{i}—Ba1—O8^{iii}	76.13 (10)	C10—C8—N3	107.1 (4)
O2—Ba1—O8^{iii}	144.53 (10)	C10—C8—H8	126.5
O5—Ba1—O8^{iii}	65.01 (10)	N3—C8—H8	126.5
O5^{i}—Ba1—O8^{iii}	84.57 (10)	N2—C9—N3	110.7 (4)
O1^{i}—Ba1—O8^{iii}	71.12 (10)	N2—C9—H9	124.6
O1—Ba1—O8^{iii}	119.12 (9)	N3—C9—H9	124.6
O8^{ii}—Ba1—O8^{iii}	69.99 (12)	C8—C10—N2	108.5 (4)
O2^{i}—Ba1—O9	79.15 (11)	C8—C10—H10	125.8
O2—Ba1—O9	65.19 (11)	N2—C10—H10	125.8
O5—Ba1—O9	137.09 (13)	O2—C12—N1	130.9 (4)
O5^{i}—Ba1—O9	79.31 (13)	O2—C12—C13	116.0 (3)
O1^{i}—Ba1—O9	65.44 (11)	N1—C12—C13	113.1 (3)
O1—Ba1—O9	104.07 (11)	O1—C13—O3	124.8 (4)
O8^{ii}—Ba1—O9	133.93 (10)	O1—C13—C12	118.2 (3)
O8^{iii}—Ba1—O9	136.55 (10)	O3—C13—C12	117.0 (3)
O2^{i}—Ba1—O9^{i}	65.19 (11)	C12—N1—C1	122.5 (3)
O2—Ba1—O9^{i}	79.15 (11)	C12—N1—Cu2	111.6 (3)
O5—Ba1—O9^{i}	79.31 (13)	C1—N1—Cu2	125.8 (3)
O5^{i}—Ba1—O9^{i}	137.09 (13)	C9—N2—C10	106.1 (4)
O1^{i}—Ba1—O9^{i}	104.07 (11)	C9—N2—Cu2	126.5 (3)
O1—Ba1—O9^{i}	65.44 (11)	C10—N2—Cu2	127.3 (3)
O8^{ii}—Ba1—O9^{i}	136.55 (10)	C9—N3—C8	107.6 (4)
O8^{iii}—Ba1—O9^{i}	133.93 (10)	C9—N3—H3A	126.2
O9—Ba1—O9^{i}	59.89 (18)	C8—N3—H3A	126.2
O4—Cu2—N1	94.38 (13)	C13—O1—Ba1	120.4 (2)
O4—Cu2—O3	175.12 (15)	C12—O2—Ba1	125.8 (3)
N1—Cu2—O3	86.53 (13)	C13—O3—Cu2	111.5 (2)
O4—Cu2—N2	89.12 (13)	C7—O4—Cu2	131.0 (3)

N1—Cu2—N2	175.91 (14)	C7—O8—Ba1^{ii}	124.9 (3)
O3—Cu2—N2	90.17 (13)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1, −*y*+2, −*z*+2; (iii) *x*, −*y*+2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{iv}	0.86	1.95	2.804 (5)	177
O5—H5*B*···O4^{iii}	0.85	1.99	2.827 (5)	169
O5—H5*B*···O8^{iii}	0.85	2.58	3.047 (5)	116
O9—H9*A*···O8^{v}	0.95	2.08	2.915 (5)	145

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