

Poly[[aqua(μ_5 -1*H*-benzimidazole-5,6-dicarboxylato)(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato)dibarium] 4.5-hydrate]

Heng-Qiang Zhang,^a Xiu-Jun Zheng,^b Chun-Xiang Zhao^c and Seik Weng Ng^{d*}

^aDepartment of Chemistry, East China Normal University, Shanghai 200062, People's Republic of China, ^bDepartment of Chemical Engineering, Huarui College, Northeast Petroleum University, Harbin 15002, People's Republic of China, ^cDepartment of Chemistry, Zhoukou Normal University, Zhoukou 466001, People's Republic of China, and ^dDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

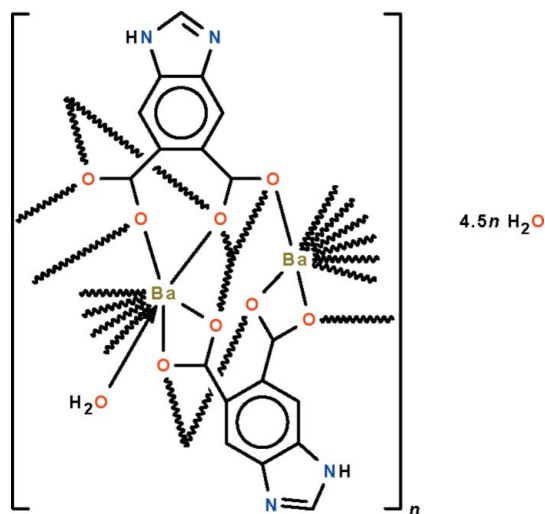
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in solvent or counterion; R factor = 0.028; wR factor = 0.074; data-to-parameter ratio = 15.3.

The polymeric title compound, $\{[\text{Ba}_2(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})] \cdot 4.5\text{H}_2\text{O}\}_n$, adopts a layer structure parallel to (001) in which adjacent Ba^{II} atoms are connected by two benzimidazole-5,6-dicarboxylate dianions, one functioning in a μ_4 -bridging mode and the other in a μ_5 -bridging mode. The Ba atom having water in its coordination environment as well as the Ba atom without water exist in a nine-coordinate polyhedron of O atoms; the geometry is difficult to derive. Lattice water molecules occupy the space between layers and interact with the layers through $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds. *ne* of the five lattice water molecules is equally disordered around an inversion centre and shows half-occupancy.

Related literature

For the strontium 1*H*-benzimidazole-5,6-dicarboxylate derivative, see: Song *et al.* (2009).



Experimental

Crystal data

$[\text{Ba}_2(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})] \cdot 4.5\text{H}_2\text{O}$
 $M_r = 782.05$
 Triclinic, $P\bar{1}$
 $a = 6.9331$ (4) Å
 $b = 9.5950$ (4) Å
 $c = 18.0179$ (7) Å
 $\alpha = 103.186$ (1)°
 $\beta = 92.068$ (2)°

$\gamma = 93.032$ (2)°
 $V = 1163.94$ (9) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.44$ mm⁻¹
 $T = 293$ K
 $0.33 \times 0.24 \times 0.21$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.396$, $T_{\text{max}} = 0.532$

11398 measured reflections
 5246 independent reflections
 4749 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.074$
 $S = 1.07$
 5246 reflections
 343 parameters

30 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.68$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}w-\text{H11} \cdots \text{O4}w^{\text{i}}$	0.84	1.66	2.49 (1)	170
$\text{O1}w-\text{H12} \cdots \text{O2}w^{\text{ii}}$	0.84	1.88	2.60 (1)	143
$\text{O2}w-\text{H21} \cdots \text{N2}$	0.84	2.00	2.83 (1)	168
$\text{O2}w-\text{H22} \cdots \text{N2}^{\text{iii}}$	0.84	2.28	2.83 (1)	124
$\text{O3}w-\text{H31} \cdots \text{N3}$	0.84	2.34	2.95 (1)	129
$\text{O3}w-\text{H32} \cdots \text{O6}w^{\text{iv}}$	0.84	1.85	2.68 (1)	174
$\text{O4}w-\text{H41} \cdots \text{O3}w^{\text{v}}$	0.84	2.03	2.84 (2)	161
$\text{O5}w-\text{H51} \cdots \text{O1}w^{\text{v}}$	0.84	2.31	2.75 (1)	113
$\text{O6}w-\text{H61} \cdots \text{O4}w^{\text{vi}}$	0.84	1.99	2.76 (1)	152
$\text{O6}w-\text{H62} \cdots \text{O8}$	0.84	2.09	2.86 (1)	152
$\text{N1}-\text{H1} \cdots \text{O1}w$	0.88	1.93	2.80 (1)	168
$\text{N4}-\text{H4} \cdots \text{O4}w$	0.88	1.99	2.86 (1)	167

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2280).

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supplementary materials

Acta Cryst. (2011). E67, m671-m672 [doi:10.1107/S160053681101590X]

Poly[[aqua(μ_5 -1*H*-benzimidazole-5,6-dicarboxylato)(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato)dibarium] 4.5-hydrate]

H.-Q. Zhang, X.-J. Zheng, C.-X. Zhao and S. W. Ng

Comment

The 1*H*-benzimidazole-5,6-dicarboxylate dianion affords a large number of metal salts; most of the crystal structure studies involve rare earth metals. The crystal structures of only few main group derivatives have been reported. The Sr^{II} derivative exists as a monohydrate; the metal atom is also coordinated by two water ligands in an eight-coordinate square-antiprismatic geometry. The dianion functions in a μ_4 bridging mode (Song *et al.*, 2009). The Ba^{II} analog has 4.5 lattice water molecules (Scheme I). Polymeric Ba₂(H₂O)(C₉H₄NO₄)₂·4.5H₂O adopts a layer structure in which adjacent Ba^{II} atoms are connected by two benzimidazole-5,6-dicarboxylate dianions, one functioning in a μ_4 bridging mode and the other in a μ_5 bridging mode. The Ba atom having water in its coordination environment as well as the Ba atom without water exist in a nine-coordinate polyhedron of O atom; the geometry is undefined. Lattice water molecules occupy the space between layers, and interact with the layers through O–H \cdots O and N–H \cdots O hydrogen bonds to generate a three-dimensional network (Table 1).

Experimental

Barium chloride (0.0416 g, 0.20 mmol) and 1*H*-benzimidazole-5,6-dicarboxylic acid (0.0412 g, 0.20 mmol) were placed in water (35 ml); the reactants dissolved upon addition of several drops of dilute sodium hydroxide to a pH of 7. The solution was set aside for the growth of crystals over several weeks; yield 60% based on Ba.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2U_{eq}(C)$. The amino and water H atoms were placed in chemically sensible positions on the basis of hydrogen bonding interactions (O–H 0.84 Å and N–H 0.88 Å); their temperature factors were tied by a factor of 1.2–1.5 times. Positioning the H atoms lead to H12 \cdots H21 and H31 \cdots H42 distances of about 2 Å, which are regarded as being acceptable. The O5w molecule then forms only one hydrogen bond. Positioning the second H atom elsewhere led to too short interactions.

On this basis, the N1 and N4 atoms are atoms having a hydrogen connected to them whereas the N2 and N3 atoms do not.

One of the water molecules (O5w) is disordered about a center-of-inversion.

The anisotropic temperature factors of the free water molecules were restrained to be nearly isotropic.

The final difference Fourier map had peaks in the vicinity of both Ba atoms.

Figures

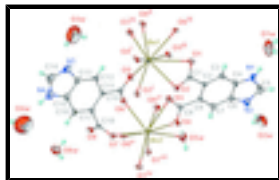


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a portion of the layer structure of $\text{Ba}_2(\text{H}_2\text{O})(\text{C}_9\text{H}_4\text{NO}_4)_2 \cdot 4.5\text{H}_2\text{O}$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Symmetry code: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x, y + 1, z$; (iv) $x, y - 1, z$; (v) $-x + 1, -y, -z + 1$; (vi) $-x, -y, -z + 1$.

Poly[[aqua(μ_5 -1*H*-benzimidazole-5,6-dicarboxylato)(μ_4 -1*H*- benzimidazole-5,6-dicarboxylato)dibarium] 4.5-hydrate]

Crystal data

$[\text{Ba}_2(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})] \cdot 4.5\text{H}_2\text{O}$	$Z = 2$
$M_r = 782.05$	$F(000) = 750$
Triclinic, $P\bar{1}$	$D_x = 2.231 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.9331 (4) \text{ \AA}$	Cell parameters from 10107 reflections
$b = 9.5950 (4) \text{ \AA}$	$\theta = 3.1\text{--}27.5^\circ$
$c = 18.0179 (7) \text{ \AA}$	$\mu = 3.44 \text{ mm}^{-1}$
$\alpha = 103.186 (1)^\circ$	$T = 293 \text{ K}$
$\beta = 92.068 (2)^\circ$	Prism, colorless
$\gamma = 93.032 (2)^\circ$	$0.33 \times 0.24 \times 0.21 \text{ mm}$
$V = 1163.94 (9) \text{ \AA}^3$	

Data collection

Rigaku R-Axis RAPID diffractometer	5246 independent reflections
Radiation source: fine-focus sealed tube graphite	4749 reflections with $I > 2\sigma(I)$
Detector resolution: $10.000 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.025$
ω scans	$\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 3.1^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.396, T_{\text{max}} = 0.532$	$k = -11 \rightarrow 12$
11398 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.074$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 1.7294P]$

5246 reflections

343 parameters

30 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\text{max}} = 1.54 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.68 \text{ e } \text{\AA}^{-3}$$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ba1	0.26276 (3)	0.610140 (19)	0.450910 (11)	0.02043 (7)	
Ba2	0.26062 (3)	0.078630 (18)	0.581428 (11)	0.01842 (7)	
O1	0.1686 (4)	0.8140 (3)	0.60189 (15)	0.0296 (5)	
O2	0.0501 (4)	0.5894 (3)	0.57721 (14)	0.0267 (5)	
O3	0.3591 (4)	0.3818 (3)	0.61724 (16)	0.0335 (6)	
O4	0.0593 (4)	0.3350 (3)	0.64668 (16)	0.0325 (6)	
O5	0.4310 (4)	0.3577 (2)	0.43836 (15)	0.0282 (5)	
O6	0.4612 (3)	0.1417 (2)	0.46119 (14)	0.0228 (5)	
O7	0.1291 (3)	-0.0557 (3)	0.43544 (14)	0.0259 (5)	
O8	0.3566 (3)	-0.1786 (3)	0.37175 (15)	0.0262 (5)	
O1w	0.3097 (12)	1.1921 (6)	0.8946 (3)	0.128 (2)	
H11	0.2025	1.2235	0.9081	0.192*	
H12	0.3998	1.2440	0.9213	0.192*	
O2w	0.5133 (16)	0.5633 (9)	1.0382 (5)	0.083 (3)	0.50
H21	0.4591	0.5883	1.0013	0.124*	0.50
H22	0.5884	0.4986	1.0218	0.124*	0.50
O3w	0.2112 (15)	0.4994 (10)	0.1075 (5)	0.177 (4)	
H31	0.1689	0.4135	0.0922	0.266*	
H32	0.2282	0.5210	0.1552	0.266*	
O4w	-0.0138 (16)	-0.3037 (13)	0.0517 (7)	0.225 (5)	
H41	0.0288	-0.3661	0.0729	0.337*	
H42	-0.0152	-0.3286	0.0039	0.337*	
O5w	0.3529 (5)	0.1624 (4)	0.74063 (18)	0.0466 (8)	
H51	0.2820	0.1137	0.7634	0.070*	
H52	0.4694	0.1486	0.7492	0.070*	
O6w	0.2361 (6)	-0.4351 (4)	0.2606 (3)	0.0666 (11)	
H61	0.1264	-0.4298	0.2790	0.100*	
H62	0.3069	-0.3650	0.2855	0.100*	
N1	0.3285 (6)	0.9029 (4)	0.8973 (2)	0.0397 (8)	
H1	0.3280	0.9966	0.9036	0.048*	
N2	0.3607 (6)	0.6883 (4)	0.9229 (2)	0.0424 (9)	
N3	0.2152 (6)	0.2189 (5)	0.1479 (2)	0.0434 (9)	
N4	0.1238 (6)	-0.0140 (5)	0.1170 (2)	0.0473 (10)	
H4	0.0825	-0.0992	0.0897	0.057*	
C1	0.1336 (4)	0.6990 (3)	0.62169 (19)	0.0198 (6)	
C2	0.1978 (5)	0.6878 (3)	0.70029 (19)	0.0199 (6)	
C3	0.2313 (5)	0.8127 (4)	0.7571 (2)	0.0250 (7)	
H3A	0.2173	0.9023	0.7467	0.030*	
C4	0.2863 (6)	0.7997 (4)	0.8300 (2)	0.0290 (7)	
C5	0.3694 (7)	0.8313 (5)	0.9496 (2)	0.0459 (11)	

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H5	0.4014	0.8757	1.0004	0.055*
C6	0.3078 (6)	0.6659 (4)	0.8458 (2)	0.0305 (8)
C7	0.2809 (6)	0.5397 (4)	0.7887 (2)	0.0294 (8)
H7	0.2983	0.4506	0.7992	0.035*
C8	0.2277 (5)	0.5522 (3)	0.71628 (19)	0.0208 (6)
C9	0.2134 (5)	0.4149 (3)	0.6539 (2)	0.0241 (7)
C10	0.4047 (4)	0.2236 (3)	0.41961 (19)	0.0198 (6)
C11	0.3099 (5)	0.1562 (3)	0.34209 (19)	0.0201 (6)
C12	0.3057 (5)	0.2372 (4)	0.2876 (2)	0.0271 (7)
H12A	0.3482	0.3337	0.2999	0.033*
C13	0.2370 (5)	0.1713 (4)	0.2147 (2)	0.0306 (8)
C14	0.1482 (8)	0.1045 (6)	0.0937 (3)	0.0517 (12)
H14	0.1213	0.1093	0.0434	0.062*
C15	0.1772 (6)	0.0235 (4)	0.1942 (2)	0.0312 (8)
C16	0.1771 (5)	-0.0567 (4)	0.2494 (2)	0.0285 (7)
H16	0.1342	-0.1530	0.2371	0.034*
C17	0.2418 (5)	0.0098 (3)	0.32264 (19)	0.0206 (6)
C18	0.2422 (5)	-0.0791 (3)	0.38180 (19)	0.0201 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01885 (11)	0.01795 (11)	0.02441 (11)	-0.00112 (7)	-0.00104 (7)	0.00554 (8)
Ba2	0.01508 (11)	0.01541 (10)	0.02374 (11)	-0.00021 (7)	0.00126 (7)	0.00261 (8)
O1	0.0343 (14)	0.0228 (12)	0.0336 (14)	-0.0030 (10)	0.0009 (11)	0.0118 (11)
O2	0.0294 (13)	0.0237 (12)	0.0247 (12)	-0.0051 (10)	-0.0022 (10)	0.0027 (10)
O3	0.0334 (15)	0.0224 (12)	0.0429 (16)	0.0048 (10)	0.0116 (12)	0.0014 (11)
O4	0.0310 (14)	0.0199 (12)	0.0433 (15)	-0.0043 (10)	-0.0035 (11)	0.0024 (11)
O5	0.0296 (14)	0.0170 (11)	0.0360 (14)	0.0010 (10)	-0.0055 (11)	0.0032 (10)
O6	0.0206 (12)	0.0219 (11)	0.0260 (12)	-0.0023 (9)	-0.0012 (9)	0.0066 (10)
O7	0.0189 (12)	0.0325 (13)	0.0245 (12)	-0.0055 (10)	0.0009 (9)	0.0042 (10)
O8	0.0210 (12)	0.0212 (11)	0.0377 (14)	0.0022 (9)	0.0004 (10)	0.0096 (11)
O1w	0.250 (7)	0.084 (3)	0.052 (3)	0.056 (4)	-0.013 (4)	0.010 (3)
O2w	0.115 (7)	0.066 (5)	0.070 (5)	0.018 (5)	-0.021 (5)	0.024 (4)
O3w	0.222 (8)	0.179 (7)	0.139 (6)	0.058 (6)	0.037 (6)	0.036 (5)
O4w	0.220 (9)	0.245 (8)	0.216 (9)	0.008 (7)	0.022 (7)	0.067 (7)
O5w	0.049 (2)	0.0500 (18)	0.0395 (17)	0.0039 (15)	0.0036 (14)	0.0080 (15)
O6w	0.058 (2)	0.046 (2)	0.089 (3)	0.0012 (17)	0.014 (2)	0.002 (2)
N1	0.051 (2)	0.0288 (16)	0.0326 (17)	0.0046 (15)	-0.0052 (15)	-0.0057 (14)
N2	0.059 (2)	0.042 (2)	0.0234 (16)	-0.0016 (17)	-0.0061 (15)	0.0048 (15)
N3	0.039 (2)	0.062 (2)	0.0366 (19)	0.0035 (18)	-0.0018 (15)	0.0271 (19)
N4	0.052 (2)	0.061 (2)	0.0265 (17)	0.0011 (19)	-0.0085 (16)	0.0065 (18)
C1	0.0138 (14)	0.0201 (15)	0.0252 (16)	0.0012 (11)	0.0034 (12)	0.0045 (13)
C2	0.0161 (15)	0.0184 (14)	0.0244 (16)	0.0021 (11)	0.0013 (12)	0.0031 (13)
C3	0.0246 (17)	0.0189 (15)	0.0304 (18)	0.0025 (13)	0.0012 (14)	0.0028 (14)
C4	0.0298 (19)	0.0263 (17)	0.0259 (17)	0.0017 (14)	-0.0002 (14)	-0.0044 (14)
C5	0.059 (3)	0.049 (3)	0.0234 (19)	0.002 (2)	-0.0075 (18)	-0.0030 (18)
C6	0.035 (2)	0.0309 (18)	0.0237 (17)	-0.0003 (15)	-0.0015 (14)	0.0036 (15)

C7	0.037 (2)	0.0222 (16)	0.0284 (18)	0.0018 (14)	-0.0023 (15)	0.0061 (14)
C8	0.0197 (16)	0.0163 (14)	0.0248 (16)	-0.0008 (12)	0.0001 (12)	0.0021 (13)
C9	0.0289 (18)	0.0157 (14)	0.0276 (17)	0.0026 (13)	-0.0018 (13)	0.0052 (13)
C10	0.0135 (14)	0.0200 (14)	0.0258 (16)	0.0013 (11)	0.0014 (12)	0.0048 (13)
C11	0.0155 (15)	0.0179 (14)	0.0272 (16)	0.0033 (11)	0.0017 (12)	0.0051 (13)
C12	0.0228 (17)	0.0273 (17)	0.0342 (19)	0.0011 (13)	0.0021 (14)	0.0128 (15)
C13	0.0247 (18)	0.041 (2)	0.0309 (19)	0.0055 (15)	0.0008 (14)	0.0178 (17)
C14	0.049 (3)	0.079 (4)	0.030 (2)	0.004 (3)	-0.0050 (19)	0.022 (2)
C15	0.0285 (19)	0.038 (2)	0.0248 (17)	0.0024 (15)	-0.0037 (14)	0.0022 (16)
C16	0.0274 (18)	0.0265 (17)	0.0292 (18)	0.0013 (14)	-0.0015 (14)	0.0019 (15)
C17	0.0166 (15)	0.0202 (15)	0.0248 (16)	0.0026 (12)	0.0006 (12)	0.0044 (13)
C18	0.0157 (15)	0.0176 (14)	0.0258 (16)	-0.0047 (11)	-0.0032 (12)	0.0044 (13)

Geometric parameters (Å, °)

Ba1—O1	3.080 (3)	O3w—H31	0.8400
Ba1—O2	2.795 (2)	O3w—H32	0.8400
Ba1—O2 ⁱ	2.769 (2)	O4w—H41	0.8401
Ba1—O3 ⁱⁱ	2.940 (3)	O4w—H42	0.8400
Ba1—O4 ⁱ	2.936 (3)	O5w—H51	0.8401
Ba1—O5	2.711 (2)	O5w—H52	0.8400
Ba1—O5 ⁱⁱ	2.816 (3)	O6w—H61	0.8401
Ba1—O6 ⁱⁱ	3.069 (2)	O6w—H62	0.8400
Ba1—O8 ⁱⁱⁱ	2.795 (2)	N1—C5	1.318 (6)
Ba2—O1 ^{iv}	2.695 (2)	N1—C4	1.389 (5)
Ba2—O3	2.871 (3)	N1—H1	0.8800
Ba2—O4	2.923 (3)	N2—C5	1.343 (6)
Ba2—O6	2.778 (2)	N2—C6	1.389 (5)
Ba2—O6 ^v	2.928 (2)	N3—C14	1.342 (7)
Ba2—O7 ^{vi}	2.700 (2)	N3—C13	1.387 (5)
Ba2—O7	2.751 (2)	N4—C14	1.304 (7)
Ba2—O8 ^v	2.806 (2)	N4—C15	1.386 (5)
Ba2—O5w	2.836 (3)	N4—H4	0.8800
O1—C1	1.249 (4)	C1—C2	1.498 (5)
O1—Ba2 ⁱⁱⁱ	2.695 (2)	C2—C3	1.390 (5)
O2—C1	1.266 (4)	C2—C8	1.419 (4)
O2—Ba1 ⁱ	2.769 (2)	C3—C4	1.389 (5)
O3—C9	1.242 (4)	C3—H3A	0.9300
O3—Ba1 ⁱⁱ	2.940 (3)	C4—C6	1.392 (5)
O4—C9	1.266 (4)	C5—H5	0.9300
O4—Ba1 ⁱ	2.936 (3)	C6—C7	1.398 (5)
O5—C10	1.255 (4)	C7—C8	1.376 (5)
O5—Ba1 ⁱⁱ	2.816 (3)	C7—H7	0.9300
O6—C10	1.270 (4)	C8—C9	1.521 (5)
O6—Ba2 ^v	2.928 (2)	C10—C11	1.509 (5)
O6—Ba1 ⁱⁱ	3.069 (2)	C10—Ba1 ⁱⁱ	3.290 (3)

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O7—C18	1.254 (4)	C11—C12	1.384 (5)
O7—Ba2 ^{vi}	2.700 (2)	C11—C17	1.419 (4)
O8—C18	1.259 (4)	C12—C13	1.377 (5)
O8—Ba1 ^{iv}	2.795 (2)	C12—H12A	0.9300
O8—Ba2 ^v	2.806 (2)	C13—C15	1.417 (6)
O1w—H11	0.8400	C14—H14	0.9300
O1w—H12	0.8400	C15—C16	1.388 (6)
O2w—O2w ^{vii}	1.613 (18)	C16—C17	1.377 (5)
O2w—H21	0.8400	C16—H16	0.9300
O2w—H22	0.8400	C17—C18	1.510 (4)
O5—Ba1—O2 ⁱ	77.01 (8)	C10—O6—Ba2	124.7 (2)
O5—Ba1—O2	95.97 (8)	C10—O6—Ba2 ^v	125.3 (2)
O2 ⁱ —Ba1—O2	64.13 (8)	Ba2—O6—Ba2 ^v	107.25 (7)
O5—Ba1—O8 ⁱⁱⁱ	126.34 (8)	C10—O6—Ba1 ⁱⁱ	88.47 (18)
O2 ⁱ —Ba1—O8 ⁱⁱⁱ	127.94 (7)	Ba2—O6—Ba1 ⁱⁱ	99.88 (7)
O2—Ba1—O8 ⁱⁱⁱ	136.76 (7)	Ba2 ^v —O6—Ba1 ⁱⁱ	99.38 (7)
O5—Ba1—O5 ⁱⁱ	70.23 (8)	C18—O7—Ba2 ^{vi}	125.1 (2)
O2 ⁱ —Ba1—O5 ⁱⁱ	128.53 (7)	C18—O7—Ba2	121.1 (2)
O2—Ba1—O5 ⁱⁱ	80.81 (8)	Ba2 ^{vi} —O7—Ba2	112.68 (8)
O8 ⁱⁱⁱ —Ba1—O5 ⁱⁱ	103.49 (7)	C18—O8—Ba1 ^{iv}	113.3 (2)
O5—Ba1—O4 ⁱ	126.10 (7)	C18—O8—Ba2 ^v	112.42 (19)
O2 ⁱ —Ba1—O4 ⁱ	63.11 (7)	Ba1 ^{iv} —O8—Ba2 ^v	106.20 (8)
O2—Ba1—O4 ⁱ	97.43 (8)	H11—O1w—H12	110.0
O8 ⁱⁱⁱ —Ba1—O4 ⁱ	66.63 (7)	O2w ^{vii} —O2w—H21	66.4
O5 ⁱⁱ —Ba1—O4 ⁱ	163.60 (7)	O2w ^{vii} —O2w—H22	51.6
O5—Ba1—O3 ⁱⁱ	68.84 (7)	H21—O2w—H22	109.5
O2 ⁱ —Ba1—O3 ⁱⁱ	132.66 (7)	H31—O3w—H32	110.7
O2—Ba1—O3 ⁱⁱ	148.68 (8)	H41—O4w—H42	112.7
O8 ⁱⁱⁱ —Ba1—O3 ⁱⁱ	60.17 (7)	Ba2—O5w—H51	109.4
O5 ⁱⁱ —Ba1—O3 ⁱⁱ	68.41 (8)	Ba2—O5w—H52	109.5
O4 ⁱ —Ba1—O3 ⁱⁱ	113.72 (8)	H51—O5w—H52	109.5
O5—Ba1—O6 ⁱⁱ	110.03 (7)	H61—O6w—H62	107.7
O2 ⁱ —Ba1—O6 ⁱⁱ	158.74 (6)	C5—N1—C4	105.7 (4)
O2—Ba1—O6 ⁱⁱ	94.83 (7)	C5—N1—H1	127.1
O8 ⁱⁱⁱ —Ba1—O6 ⁱⁱ	64.97 (7)	C4—N1—H1	127.1
O5 ⁱⁱ —Ba1—O6 ⁱⁱ	44.11 (6)	C5—N2—C6	105.2 (4)
O4 ⁱ —Ba1—O6 ⁱⁱ	120.42 (7)	C14—N3—C13	106.3 (4)
O3 ⁱⁱ —Ba1—O6 ⁱⁱ	67.22 (7)	C14—N4—C15	105.0 (4)
O5—Ba1—O1	125.39 (7)	C14—N4—H4	127.5
O2 ⁱ —Ba1—O1	103.10 (7)	C15—N4—H4	127.5
O2—Ba1—O1	43.78 (6)	O1—C1—O2	122.6 (3)
O8 ⁱⁱⁱ —Ba1—O1	97.04 (7)	O1—C1—C2	119.2 (3)

O5 ⁱⁱ —Ba1—O1	68.40 (7)	O2—C1—C2	118.2 (3)
O4 ⁱ —Ba1—O1	98.98 (7)	C3—C2—C8	120.4 (3)
O3 ⁱⁱ —Ba1—O1	123.17 (7)	C3—C2—C1	118.9 (3)
O6 ⁱⁱ —Ba1—O1	56.15 (6)	C8—C2—C1	120.7 (3)
O1 ^{iv} —Ba2—O7 ^{vi}	76.72 (8)	C4—C3—C2	118.0 (3)
O1 ^{iv} —Ba2—O7	80.25 (8)	C4—C3—H3A	121.0
O7 ^{vi} —Ba2—O7	67.32 (8)	C2—C3—H3A	121.0
O1 ^{iv} —Ba2—O6	125.88 (8)	C3—C4—N1	131.1 (4)
O7 ^{vi} —Ba2—O6	116.89 (7)	C3—C4—C6	121.1 (3)
O7—Ba2—O6	62.22 (7)	N1—C4—C6	107.7 (3)
O1 ^{iv} —Ba2—O8 ^v	113.68 (8)	N1—C5—N2	113.9 (4)
O7 ^{vi} —Ba2—O8 ^v	163.12 (8)	N1—C5—H5	123.1
O7—Ba2—O8 ^v	126.06 (7)	N2—C5—H5	123.1
O6—Ba2—O8 ^v	68.87 (7)	N2—C6—C4	107.4 (3)
O1 ^{iv} —Ba2—O5w	87.21 (9)	N2—C6—C7	131.1 (4)
O7 ^{vi} —Ba2—O5w	106.45 (9)	C4—C6—C7	121.4 (3)
O7—Ba2—O5w	166.97 (8)	C8—C7—C6	117.6 (3)
O6—Ba2—O5w	129.48 (9)	C8—C7—H7	121.2
O8 ^v —Ba2—O5w	62.57 (9)	C6—C7—H7	121.2
O1 ^{iv} —Ba2—O3	159.72 (8)	C7—C8—C2	121.4 (3)
O7 ^{vi} —Ba2—O3	104.58 (8)	C7—C8—C9	116.6 (3)
O7—Ba2—O3	119.27 (8)	C2—C8—C9	121.9 (3)
O6—Ba2—O3	72.16 (7)	O3—C9—O4	123.7 (3)
O8 ^v —Ba2—O3	60.90 (8)	O3—C9—C8	118.1 (3)
O5w—Ba2—O3	72.92 (9)	O4—C9—C8	118.0 (3)
O1 ^{iv} —Ba2—O4	124.90 (8)	O5—C10—O6	123.3 (3)
O7 ^{vi} —Ba2—O4	63.37 (7)	O5—C10—C11	118.2 (3)
O7—Ba2—O4	113.76 (8)	O6—C10—C11	118.4 (3)
O6—Ba2—O4	106.09 (7)	O5—C10—Ba1 ⁱⁱ	57.20 (18)
O8 ^v —Ba2—O4	100.03 (7)	O6—C10—Ba1 ⁱⁱ	68.83 (18)
O5w—Ba2—O4	70.81 (9)	C11—C10—Ba1 ⁱⁱ	159.4 (2)
O3—Ba2—O4	44.87 (7)	C12—C11—C17	120.1 (3)
O1 ^{iv} —Ba2—O6 ^v	61.79 (7)	C12—C11—C10	118.3 (3)
O7 ^{vi} —Ba2—O6 ^v	129.53 (7)	C17—C11—C10	121.3 (3)
O7—Ba2—O6 ^v	77.96 (7)	C13—C12—C11	118.3 (3)
O6—Ba2—O6 ^v	72.75 (7)	C13—C12—H12A	120.9
O8 ^v —Ba2—O6 ^v	66.84 (7)	C11—C12—H12A	120.9
O5w—Ba2—O6 ^v	99.26 (8)	C12—C13—N3	133.1 (4)
O3—Ba2—O6 ^v	124.42 (7)	C12—C13—C15	121.7 (3)
O4—Ba2—O6 ^v	166.54 (7)	N3—C13—C15	105.1 (4)
C1—O1—Ba2 ⁱⁱⁱ	171.4 (2)	N4—C14—N3	114.6 (4)
C1—O1—Ba1	82.76 (19)	N4—C14—H14	122.7

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Ba2 ⁱⁱⁱ —O1—Ba1	104.56 (8)	N3—C14—H14	122.7
C1—O2—Ba1 ⁱ	147.4 (2)	N4—C15—C16	131.3 (4)
C1—O2—Ba1	95.42 (19)	N4—C15—C13	108.9 (4)
Ba1 ⁱ —O2—Ba1	115.87 (8)	C16—C15—C13	119.9 (3)
C9—O3—Ba2	95.3 (2)	C17—C16—C15	118.4 (3)
C9—O3—Ba1 ⁱⁱ	163.6 (2)	C17—C16—H16	120.8
Ba2—O3—Ba1 ⁱⁱ	100.86 (8)	C15—C16—H16	120.8
C9—O4—Ba2	92.3 (2)	C16—C17—C11	121.5 (3)
C9—O4—Ba1 ⁱ	118.6 (2)	C16—C17—C18	117.8 (3)
Ba2—O4—Ba1 ⁱ	114.25 (9)	C11—C17—C18	120.7 (3)
C10—O5—Ba1	145.3 (2)	O7—C18—O8	123.6 (3)
C10—O5—Ba1 ⁱⁱ	100.8 (2)	O7—C18—C17	120.6 (3)
Ba1—O5—Ba1 ⁱⁱ	109.77 (8)	O8—C18—C17	115.8 (3)
O5—Ba1—O1—C1	-35.8 (2)	O3—Ba2—O7—C18	74.1 (3)
O2 ⁱ —Ba1—O1—C1	47.5 (2)	O4—Ba2—O7—C18	124.3 (2)
O2—Ba1—O1—C1	20.40 (18)	O6 ^v —Ba2—O7—C18	-48.8 (2)
O8 ⁱⁱⁱ —Ba1—O1—C1	179.1 (2)	O1 ^{iv} —Ba2—O7—Ba2 ^{vi}	79.59 (10)
O5 ⁱⁱ —Ba1—O1—C1	-79.1 (2)	O7 ^{vi} —Ba2—O7—Ba2 ^{vi}	0.0
O4 ⁱ —Ba1—O1—C1	111.8 (2)	O6—Ba2—O7—Ba2 ^{vi}	-140.71 (12)
O3 ⁱⁱ —Ba1—O1—C1	-122.06 (19)	O8 ^v —Ba2—O7—Ba2 ^{vi}	-168.15 (7)
O6 ⁱⁱ —Ba1—O1—C1	-127.5 (2)	O5 ^w —Ba2—O7—Ba2 ^{vi}	63.6 (4)
O5—Ba1—O1—Ba2 ⁱⁱⁱ	139.56 (8)	O3—Ba2—O7—Ba2 ^{vi}	-94.51 (10)
O2 ⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	-137.20 (9)	O4—Ba2—O7—Ba2 ^{vi}	-44.37 (11)
O2—Ba1—O1—Ba2 ⁱⁱⁱ	-164.28 (15)	O6 ^v —Ba2—O7—Ba2 ^{vi}	142.60 (10)
O8 ⁱⁱⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	-5.53 (9)	Ba1—O1—C1—O2	-39.2 (3)
O5 ⁱⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	96.23 (9)	Ba1—O1—C1—C2	138.9 (3)
O4 ⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	-72.88 (9)	Ba1 ⁱ —O2—C1—O1	-120.1 (4)
O3 ⁱⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	53.27 (12)	Ba1—O2—C1—O1	44.0 (3)
O6 ⁱⁱ —Ba1—O1—Ba2 ⁱⁱⁱ	47.87 (8)	Ba1 ⁱ —O2—C1—C2	61.8 (5)
O5—Ba1—O2—C1	117.0 (2)	Ba1—O2—C1—C2	-134.1 (2)
O2 ⁱ —Ba1—O2—C1	-170.5 (3)	O1—C1—C2—C3	22.3 (5)
O8 ⁱⁱⁱ —Ba1—O2—C1	-51.7 (2)	O2—C1—C2—C3	-159.5 (3)
O5 ⁱⁱ —Ba1—O2—C1	48.2 (2)	O1—C1—C2—C8	-156.5 (3)
O4 ⁱ —Ba1—O2—C1	-115.3 (2)	O2—C1—C2—C8	21.7 (5)
O3 ⁱⁱ —Ba1—O2—C1	58.8 (3)	C8—C2—C3—C4	-2.7 (5)
O6 ⁱⁱ —Ba1—O2—C1	6.3 (2)	C1—C2—C3—C4	178.5 (3)
O1—Ba1—O2—C1	-20.05 (18)	C2—C3—C4—N1	-179.8 (4)
O5—Ba1—O2—Ba1 ⁱ	-72.43 (10)	C2—C3—C4—C6	0.2 (6)
O2 ⁱ —Ba1—O2—Ba1 ⁱ	0.0	C5—N1—C4—C3	179.1 (4)
O8 ⁱⁱⁱ —Ba1—O2—Ba1 ⁱ	118.81 (11)	C5—N1—C4—C6	-0.9 (5)
O5 ⁱⁱ —Ba1—O2—Ba1 ⁱ	-141.24 (11)	C4—N1—C5—N2	0.8 (6)
O4 ⁱ —Ba1—O2—Ba1 ⁱ	55.24 (10)	C6—N2—C5—N1	-0.4 (6)

O3 ⁱⁱ —Ba1—O2—Ba1 ⁱ	-130.67 (12)	C5—N2—C6—C4	-0.3 (5)
O6 ⁱⁱ —Ba1—O2—Ba1 ⁱ	176.81 (9)	C5—N2—C6—C7	178.3 (5)
O1—Ba1—O2—Ba1 ⁱ	150.49 (16)	C3—C4—C6—N2	-179.3 (4)
O1 ^{iv} —Ba2—O3—C9	-57.0 (4)	N1—C4—C6—N2	0.7 (5)
O7 ^{vi} —Ba2—O3—C9	34.1 (2)	C3—C4—C6—C7	2.0 (6)
O7—Ba2—O3—C9	106.0 (2)	N1—C4—C6—C7	-178.0 (4)
O6—Ba2—O3—C9	148.1 (2)	N2—C6—C7—C8	-179.9 (4)
O8 ^v —Ba2—O3—C9	-136.6 (2)	C4—C6—C7—C8	-1.5 (6)
O5 ^w —Ba2—O3—C9	-69.0 (2)	C6—C7—C8—C2	-1.1 (5)
O4—Ba2—O3—C9	10.7 (2)	C6—C7—C8—C9	175.7 (3)
O6 ^v —Ba2—O3—C9	-158.6 (2)	C3—C2—C8—C7	3.2 (5)
O1 ^{iv} —Ba2—O3—Ba1 ⁱⁱ	120.0 (2)	C1—C2—C8—C7	-178.0 (3)
O7 ^{vi} —Ba2—O3—Ba1 ⁱⁱ	-148.87 (8)	C3—C2—C8—C9	-173.4 (3)
O7—Ba2—O3—Ba1 ⁱⁱ	-76.98 (10)	C1—C2—C8—C9	5.4 (5)
O6—Ba2—O3—Ba1 ⁱⁱ	-34.84 (8)	Ba2—O3—C9—O4	-21.3 (4)
O8 ^v —Ba2—O3—Ba1 ⁱⁱ	40.43 (8)	Ba1 ⁱⁱ —O3—C9—O4	169.0 (7)
O5 ^w —Ba2—O3—Ba1 ⁱⁱ	108.05 (11)	Ba2—O3—C9—C8	152.6 (3)
O4—Ba2—O3—Ba1 ⁱⁱ	-172.25 (15)	Ba1 ⁱⁱ —O3—C9—C8	-17.2 (11)
O6 ^v —Ba2—O3—Ba1 ⁱⁱ	18.42 (12)	Ba2—O4—C9—O3	20.8 (4)
O1 ^{iv} —Ba2—O4—C9	146.5 (2)	Ba1 ⁱ —O4—C9—O3	-98.5 (4)
O7 ^{vi} —Ba2—O4—C9	-165.0 (2)	Ba2—O4—C9—C8	-153.0 (3)
O7—Ba2—O4—C9	-118.8 (2)	Ba1 ⁱ —O4—C9—C8	87.6 (3)
O6—Ba2—O4—C9	-52.6 (2)	C7—C8—C9—O3	-91.7 (4)
O8 ^v —Ba2—O4—C9	18.2 (2)	C2—C8—C9—O3	85.1 (4)
O5 ^w —Ba2—O4—C9	74.3 (2)	C7—C8—C9—O4	82.5 (4)
O3—Ba2—O4—C9	-10.4 (2)	C2—C8—C9—O4	-100.7 (4)
O6 ^v —Ba2—O4—C9	30.6 (4)	Ba1—O5—C10—O6	-131.3 (3)
O1 ^{iv} —Ba2—O4—Ba1 ⁱ	-90.55 (11)	Ba1 ⁱⁱ —O5—C10—O6	20.4 (4)
O7 ^{vi} —Ba2—O4—Ba1 ⁱ	-42.08 (8)	Ba1—O5—C10—C11	51.7 (5)
O7—Ba2—O4—Ba1 ⁱ	4.13 (11)	Ba1 ⁱⁱ —O5—C10—C11	-156.6 (2)
O6—Ba2—O4—Ba1 ⁱ	70.37 (10)	Ba1—O5—C10—Ba1 ⁱⁱ	-151.7 (4)
O8 ^v —Ba2—O4—Ba1 ⁱ	141.10 (9)	Ba2—O6—C10—O5	82.7 (4)
O5 ^w —Ba2—O4—Ba1 ⁱ	-162.74 (12)	Ba2 ^v —O6—C10—O5	-118.7 (3)
O3—Ba2—O4—Ba1 ⁱ	112.48 (14)	Ba1 ⁱⁱ —O6—C10—O5	-18.3 (3)
O6 ^v —Ba2—O4—Ba1 ⁱ	153.5 (2)	Ba2—O6—C10—C11	-100.4 (3)
O2 ⁱ —Ba1—O5—C10	10.7 (4)	Ba2 ^v —O6—C10—C11	58.2 (3)
O2—Ba1—O5—C10	72.3 (4)	Ba1 ⁱⁱ —O6—C10—C11	158.7 (3)
O8 ⁱⁱⁱ —Ba1—O5—C10	-117.2 (4)	Ba2—O6—C10—Ba1 ⁱⁱ	100.96 (18)
O5 ⁱⁱ —Ba1—O5—C10	150.3 (5)	Ba2 ^v —O6—C10—Ba1 ⁱⁱ	-100.42 (18)
O4 ⁱ —Ba1—O5—C10	-31.4 (4)	O5—C10—C11—C12	17.9 (5)
O3 ⁱⁱ —Ba1—O5—C10	-136.0 (4)	O6—C10—C11—C12	-159.2 (3)
O6 ⁱⁱ —Ba1—O5—C10	169.7 (4)	Ba1 ⁱⁱ —C10—C11—C12	-53.5 (7)

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O1—Ba1—O5—C10	107.6 (4)	O5—C10—C11—C17	-167.7 (3)
O2 ⁱ —Ba1—O5—Ba1 ⁱⁱ	-139.66 (10)	O6—C10—C11—C17	15.2 (5)
O2—Ba1—O5—Ba1 ⁱⁱ	-77.98 (9)	Ba1 ⁱⁱ —C10—C11—C17	121.0 (5)
O8 ⁱⁱⁱ —Ba1—O5—Ba1 ⁱⁱ	92.48 (11)	C17—C11—C12—C13	-1.0 (5)
O5 ⁱⁱ —Ba1—O5—Ba1 ⁱⁱ	0.0	C10—C11—C12—C13	173.5 (3)
O4 ⁱ —Ba1—O5—Ba1 ⁱⁱ	178.30 (8)	C11—C12—C13—N3	-179.2 (4)
O3 ⁱⁱ —Ba1—O5—Ba1 ⁱⁱ	73.73 (10)	C11—C12—C13—C15	-2.0 (6)
O6 ⁱⁱ —Ba1—O5—Ba1 ⁱⁱ	19.40 (11)	C14—N3—C13—C12	177.3 (5)
O1—Ba1—O5—Ba1 ⁱⁱ	-42.68 (12)	C14—N3—C13—C15	-0.2 (5)
O1 ^{iv} —Ba2—O6—C10	128.5 (2)	C15—N4—C14—N3	0.6 (6)
O7 ^{vi} —Ba2—O6—C10	35.7 (3)	C13—N3—C14—N4	-0.2 (6)
O7—Ba2—O6—C10	76.6 (2)	C14—N4—C15—C16	178.2 (5)
O8 ^v —Ba2—O6—C10	-126.9 (3)	C14—N4—C15—C13	-0.7 (5)
O5 ^w —Ba2—O6—C10	-110.3 (3)	C12—C13—C15—N4	-177.3 (4)
O3—Ba2—O6—C10	-62.0 (2)	N3—C13—C15—N4	0.6 (5)
O4—Ba2—O6—C10	-32.2 (3)	C12—C13—C15—C16	3.6 (6)
O6 ^v —Ba2—O6—C10	161.8 (3)	N3—C13—C15—C16	-178.5 (4)
O1 ^{iv} —Ba2—O6—Ba2 ^v	-33.33 (12)	N4—C15—C16—C17	179.1 (4)
O7 ^{vi} —Ba2—O6—Ba2 ^v	-126.14 (8)	C13—C15—C16—C17	-2.1 (6)
O7—Ba2—O6—Ba2 ^v	-85.22 (9)	C15—C16—C17—C11	-0.8 (5)
O8 ^v —Ba2—O6—Ba2 ^v	71.25 (8)	C15—C16—C17—C18	-179.5 (3)
O5 ^w —Ba2—O6—Ba2 ^v	87.86 (12)	C12—C11—C17—C16	2.4 (5)
O3—Ba2—O6—Ba2 ^v	136.20 (10)	C10—C11—C17—C16	-171.9 (3)
O4—Ba2—O6—Ba2 ^v	165.99 (7)	C12—C11—C17—C18	-178.9 (3)
O6 ^v —Ba2—O6—Ba2 ^v	0.0	C10—C11—C17—C18	6.8 (5)
O1 ^{iv} —Ba2—O6—Ba1 ⁱⁱ	-136.47 (8)	Ba2 ^{vi} —O7—C18—O8	-115.8 (3)
O7 ^{vi} —Ba2—O6—Ba1 ⁱⁱ	130.72 (7)	Ba2—O7—C18—O8	77.0 (4)
O7—Ba2—O6—Ba1 ⁱⁱ	171.65 (10)	Ba2 ^{vi} —O7—C18—C17	61.7 (4)
O8 ^v —Ba2—O6—Ba1 ⁱⁱ	-31.89 (7)	Ba2—O7—C18—C17	-105.5 (3)
O5 ^w —Ba2—O6—Ba1 ⁱⁱ	-15.28 (13)	Ba1 ^{iv} —O8—C18—O7	17.2 (4)
O3—Ba2—O6—Ba1 ⁱⁱ	33.06 (8)	Ba2 ^v —O8—C18—O7	-103.3 (3)
O4—Ba2—O6—Ba1 ⁱⁱ	62.86 (8)	Ba1 ^{iv} —O8—C18—C17	-160.4 (2)
O6 ^v —Ba2—O6—Ba1 ⁱⁱ	-103.13 (9)	Ba2 ^v —O8—C18—C17	79.1 (3)
O1 ^{iv} —Ba2—O7—C18	-111.8 (3)	C16—C17—C18—O7	-112.0 (4)
O7 ^{vi} —Ba2—O7—C18	168.6 (3)	C11—C17—C18—O7	69.3 (4)
O6—Ba2—O7—C18	27.9 (2)	C16—C17—C18—O8	65.7 (4)
O8 ^v —Ba2—O7—C18	0.5 (3)	C11—C17—C18—O8	-113.0 (3)
O5 ^w —Ba2—O7—C18	-127.7 (4)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1w—H11···O4w ⁱ	0.84	1.66	2.49 (1)	170
O1w—H12···O2w ^{viii}	0.84	1.88	2.60 (1)	143
O2w—H21···N2	0.84	2.00	2.83 (1)	168
O2w—H22···N2 ^{vii}	0.84	2.28	2.83 (1)	124
O3w—H31···N3	0.84	2.34	2.95 (1)	129
O3w—H32···O6w ⁱⁱⁱ	0.84	1.85	2.68 (1)	174
O4w—H41···O3w ^{iv}	0.84	2.03	2.84 (2)	161
O5w—H51···O1w ^{iv}	0.84	2.31	2.75 (1)	113
O6w—H61···O4 ^{vi}	0.84	1.99	2.76 (1)	152
O6w—H62···O8	0.84	2.09	2.86 (1)	152
N1—H1···O1w	0.88	1.93	2.80 (1)	168
N4—H4···O4w	0.88	1.99	2.86 (1)	167

Symmetry codes: (i) $-x, -y+1, -z+1$; (viii) $-x+1, -y+2, -z+2$; (vii) $-x+1, -y+1, -z+2$; (iii) $x, y+1, z$; (iv) $x, y-1, z$; (vi) $-x, -y, -z+1$.

Fig. 1

