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Poly[μ_6-pyridine-2,4-dicarboxylato-barium]

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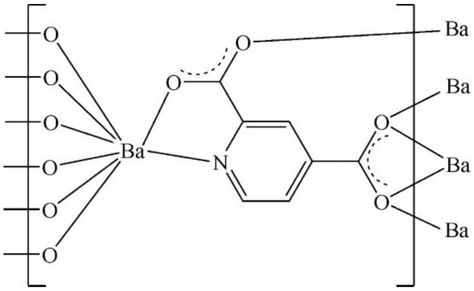
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.018; wR factor = 0.048; data-to-parameter ratio = 14.0.

In the title complex, $[Ba(C_7H_3NO_4)]_n$, the coordination geometry around the Ba^{II} ion can be described as a distorted bicapped trigonal-prismatic $BaNO_7$ arrangement. The pyridine-2,4-dicarboxylic acid ligands exhibit a new coordination mode. Adjacent metal centers are linked by the O atoms of the pyridine-2,4-dicarboxylic acid ligands, and then form a three-dimensional supramolecular polymeric framework.

Related literature

For related structures, see: Frisch & Cahill (2006); Huang *et al.* (2007); Li *et al.* (2008); Liang *et al.* (2002); Noro *et al.* (2002); Soleimannejad *et al.* (2009); Zhang (2005).



Experimental

Crystal data

$[Ba(C_7H_3NO_4)]$	V = 1477.3 (2) Å^3
M_r = 302.44	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 11.7570 (11) Å	μ = 5.35 mm^{-1}
b = 7.2121 (7) Å	T = 296 K
c = 17.4547 (16) Å	0.37 × 0.34 × 0.07 mm
β = 93.471 (1)°	

Data collection

Bruker SMART CCD area-detector diffractometer	4192 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	1662 independent reflections
T_{min} = 0.325, T_{max} = 0.783	1547 reflections with $I > 2\sigma(I)$
	R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018	119 parameters
$wR(F^2)$ = 0.048	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
1662 reflections	$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2031).

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supporting information

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Poly[μ_6-pyridine-2,4-dicarboxylato-barium]

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S1. Comment

Complex of Sr^{II} ion with pyridine-2,4-dicarboxylic acid, [Sr($C_7H_3NO_4$)(H_2O)$_2$]$_n$, has been previously studied (Soleimannejad *et al.*, 2009), which is a two-dimensional polymer.

Here we report a complex (I) assembled by alkaline earth metal Ba^{II} ion with pyridine-2,4-dicarboxylic acid ligand. The formula for the complex is [Ba($C_7H_3NO_4$)]$_n$, X-ray crystal analyse reveals that the pyridine-2,4-dicarboxylic acid ligands in the complex are completely deprotonated, which is the same with the complex of [Sr($C_7H_3NO_4$)(H_2O)$_2$]$_n$.

In the title complex, the asymmetric unit consists of one Ba^{II} ion and one pyridine-2,4-dicarboxylate. The coordination geometry around Ba^{II} ion (Fig. 1) could be described as a distorted bicapped trigonal prism arrangement with coordination number of 8, where N1, O2B and O4D form the top plane of the trigonal prism, and the bottom plane is completed by O3A, O4E, and O1C, while O1 and O3E capped two quadrilateral faces formed by N1, O3A, O1C, O4D and O2B, O4E, O1C, O4D, respectively. All the coordinated atoms in the title complex are oxygen atoms and nitrogen atoms of pyridine-2,4-dicarboxylic acid ligands, which is different from the complex of [Sr($C_7H_3NO_4$)(H_2O)$_2$]$_n$, oxygen atoms of water molecules also take part in the coordination with metal centers. The bond length of Ba—O$_{carboxylate}$ bonds range from 2.706 (2) to 2.8941 (19) Å, which compare well with the mean value determined from the CSD [2.798 (7) Å for Ba—O$_{carboxylate}$ bond](Table 1). The coordination mode (Fig. 2) of pyridine-2,4-dicarboxylic acid ligands can be classified as μ_6-(κ^8N, O^1: O^1: O^2: O^3: O^3: O^4: O^4), that is, two 4-position carboxylate oxygen atoms (O3 and O4) coordinate to three Ba^{II} ions, one of the 2-position carboxylate oxygen atoms (O1) coordinates to two Ba^{II} ions, at the same time, this oxygen atom chelate a Ba^{II} ion with the pyridyl nitrogen (N1). The other 2-position oxygen atom (O2) coordinates to one Ba^{II} ion. This coordination mode is not observed in previous reports (Soleimannejad *et al.*, 2009; Huang *et al.*, 2007; Zhang, 2005; Liang *et al.*, 2002; Li *et al.*, 2008; Frisch *et al.*, 2006; Noro *et al.*, 2002). The adjacent metal centers are linked by the oxygen and nitrogen atoms of pyridine-2,4-dicarboxylic acid ligands, and then form a three-dimensional supramolecular polymeric framework (Fig. 3), while in the complex of Sr($C_7H_3NO_4$)(H_2O)$_2$]$_n$ (Soleimannejad *et al.*, 2009), the three-dimensional structure is constructed by non-covalent interactions consisting of O—H···O hydrogen bonds and π-π stacking interactions.

S2. Experimental

A mixture of barium chloride dihydrate (0.0244 g, 0.1 mmol), sodium hydroxide (0.0080 g, 0.2 mmol), pyridine-2,4-dicarboxylic acid (0.0167 g, 0.1 mmol), and H_2O (3 mL) was placed in a Parr Teflon-lined stainless stell vessel (25 ml), and then the vessel was sealed and heated at 443.15 K for 4 days. Then the vessel was cooled to 373.15 K at a rate of 5 K h^{-1} and slowly cooled to room temperature. Colorless, rectangular single crystals suitable for X-ray diffraction were obtained.

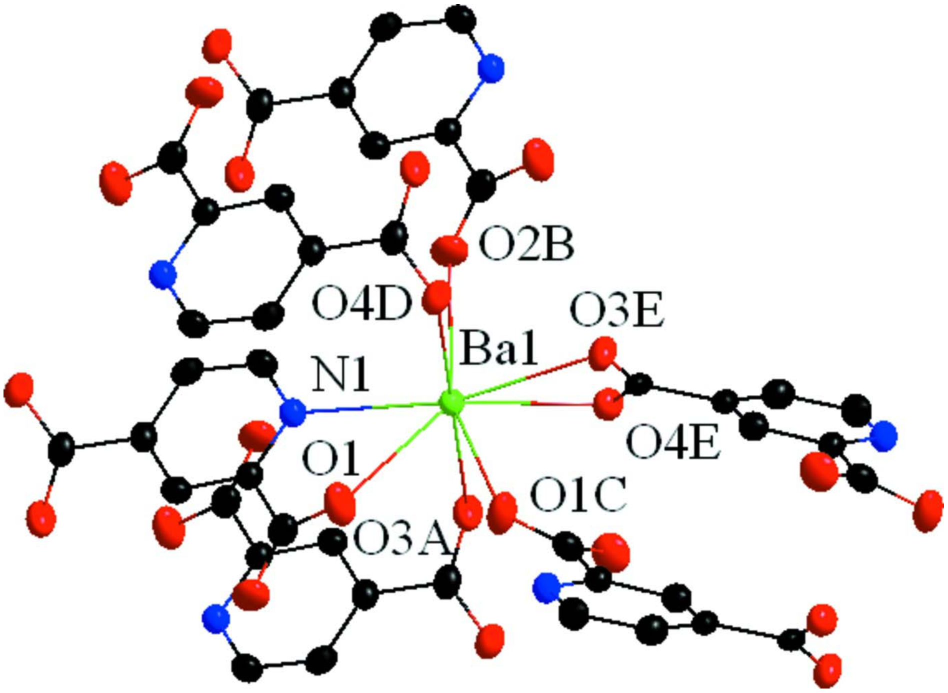

Figure 1

Coordination environment of Ba^{II} ion in the title complex. Non-hydrogen atoms are shown as 30% probability ellipsoids. Hydrogen atoms are omitted for clarity. Symmetry codes: (A) -*x* + 1, -*y*, -*z* + 1; (B) *x* - 1/2, *y* + 1/2, *z*; (C) -*x* + 1, *y*, -*z* + 1/2; (D) -*x* + 1, -*y* + 1, -*z* + 1; (E) *x* - 1/2, -*y* + 1/2, *z* - 1/2.

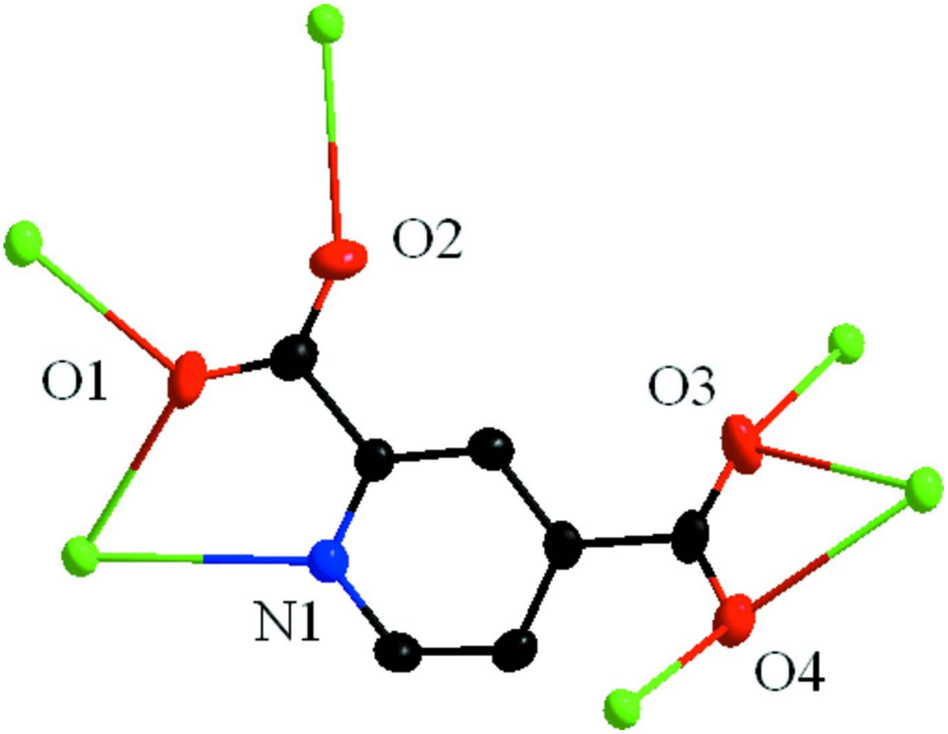

Figure 2

Coordination mode of pyridine-2,4-dicarboxylic acid ligands in the title complex. Non-hydrogen atoms are shown as 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

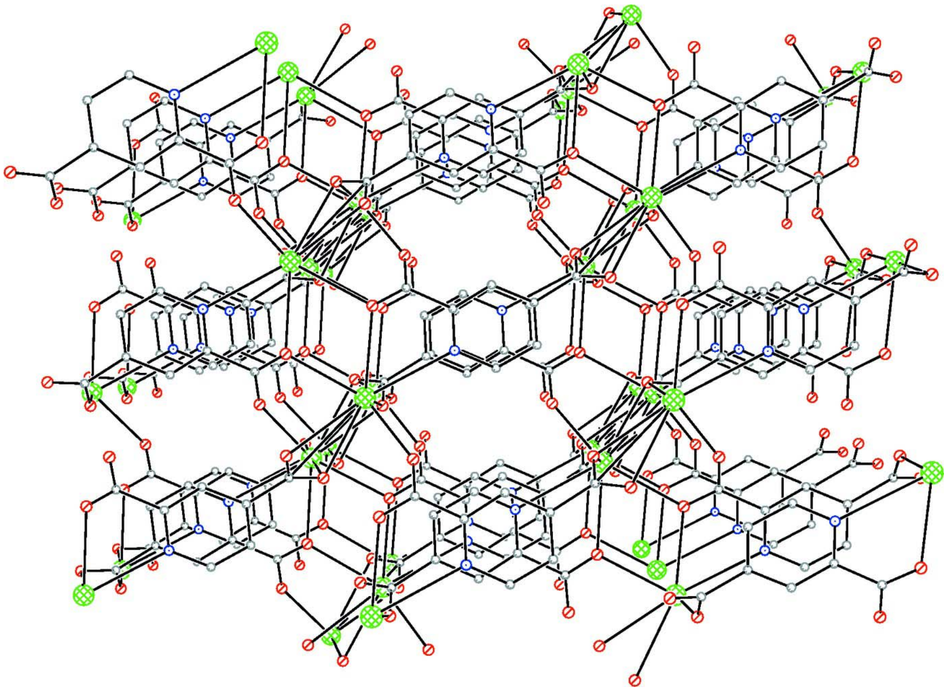

Figure 3

View of three-dimensional framework along *b* axis in the title complex.

Poly[μ_6-pyridine-2,4-dicarboxylato-barium]

Crystal data

[Ba($C_7H_3NO_4$)]
$M_r = 302.44$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 11.7570\ (11)$ Å
$b = 7.2121\ (7)$ Å
$c = 17.4547\ (16)$ Å
$\beta = 93.471\ (1)°$
$V = 1477.3\ (2)$ Å^3
$Z = 8$
$F(000) = 1120$
$D_x = 2.720$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2902 reflections
$\theta = 2.3–27.5°$
$\mu = 5.35$ mm^{-1}
$T = 296$ K
Block, colorless
0.37 × 0.34 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.325$, $T_{\max} = 0.783$
4192 measured reflections
1662 independent reflections
1547 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.018$
$\theta_{\max} = 27.5°$, $\theta_{\min} = 2.3°$
$h = -15 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.048$
$S = 1.03$
1662 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.0287P)^2 + 1.379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.70$ e Å^{-3}
$\Delta\rho_{\min} = -0.45$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00237 (13)

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 $F^2 > \sigma(F^2)$ 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}
Ba1	0.332689 (13)	0.35356 (2)	0.305017 (8)	0.01561 (9)
N1	0.44887 (19)	0.2899 (3)	0.45739 (13)	0.0175 (5)
O1	0.55983 (18)	0.2658 (3)	0.32482 (11)	0.0282 (5)

O2	0.68945 (17)	0.0756 (3)	0.38112 (12)	0.0260 (4)
O3	0.69395 (18)	0.0151 (3)	0.67349 (12)	0.0255 (4)
O4	0.63043 (17)	0.2757 (3)	0.72435 (11)	0.0214 (4)
C3	0.5531 (2)	0.2109 (4)	0.45821 (15)	0.0151 (5)
C4	0.6129 (2)	0.1626 (3)	0.52576 (17)	0.0179 (6)
H4	0.6828	0.1027	0.5245	0.021*
C5	0.5685 (2)	0.2036 (4)	0.59553 (15)	0.0162 (5)
C6	0.4620 (2)	0.2887 (4)	0.59501 (16)	0.0188 (5)
H6	0.4299	0.3208	0.6406	0.023*
C7	0.4053 (2)	0.3242 (4)	0.52447 (17)	0.0196 (6)
H7	0.3326	0.3749	0.5241	0.023*
C1	0.6053 (2)	0.1797 (4)	0.38175 (17)	0.0190 (6)
C2	0.6353 (2)	0.1607 (3)	0.67076 (16)	0.0169 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01808 (12)	0.01548 (11)	0.01308 (12)	0.00230 (5)	−0.00070 (7)	−0.00040 (5)
N1	0.0179 (11)	0.0184 (11)	0.0159 (11)	0.0011 (9)	−0.0007 (9)	−0.0004 (9)
O1	0.0256 (11)	0.0458 (13)	0.0133 (10)	0.0028 (10)	0.0015 (8)	0.0056 (9)
O2	0.0215 (10)	0.0315 (11)	0.0258 (11)	0.0039 (9)	0.0080 (8)	−0.0055 (9)
O3	0.0332 (11)	0.0187 (10)	0.0231 (11)	0.0011 (9)	−0.0093 (9)	0.0031 (8)
O4	0.0263 (10)	0.0228 (10)	0.0148 (10)	−0.0029 (8)	−0.0006 (8)	−0.0009 (8)
C3	0.0169 (12)	0.0139 (12)	0.0146 (13)	−0.0013 (10)	0.0007 (10)	0.0002 (10)
C4	0.0175 (13)	0.0161 (12)	0.0200 (14)	0.0007 (9)	0.0012 (11)	−0.0003 (10)
C5	0.0187 (13)	0.0135 (11)	0.0160 (13)	−0.0029 (10)	−0.0014 (10)	0.0026 (10)
C6	0.0234 (14)	0.0173 (12)	0.0162 (13)	−0.0002 (11)	0.0037 (10)	−0.0026 (11)
C7	0.0156 (13)	0.0212 (13)	0.0220 (15)	0.0030 (10)	0.0019 (11)	−0.0008 (11)
C1	0.0163 (13)	0.0226 (13)	0.0183 (14)	−0.0041 (11)	0.0027 (10)	−0.0019 (11)
C2	0.0204 (14)	0.0165 (13)	0.0137 (13)	−0.0066 (10)	−0.0003 (11)	0.0039 (10)

Geometric parameters (Å, º)

Ba1—O3^{i}	2.706 (2)	O3—Ba1^{i}	2.706 (2)
Ba1—O2^{ii}	2.727 (2)	O3—Ba1^{vii}	2.8941 (19)
Ba1—O1^{iii}	2.735 (2)	O4—C2	1.254 (3)
Ba1—O1	2.746 (2)	O4—Ba1^{iv}	2.762 (2)
Ba1—O4^{iv}	2.762 (2)	O4—Ba1^{vii}	2.8463 (19)
Ba1—O4^{v}	2.8463 (19)	C3—C4	1.380 (4)
Ba1—O3^{v}	2.8941 (19)	C3—C1	1.519 (4)
Ba1—N1	2.951 (2)	C4—C5	1.385 (4)
Ba1—C2^{v}	3.199 (3)	C4—H4	0.9300
N1—C7	1.329 (4)	C5—C6	1.394 (4)
N1—C3	1.351 (3)	C5—C2	1.520 (4)
O1—C1	1.263 (3)	C6—C7	1.388 (4)
O1—Ba1^{iii}	2.735 (2)	C6—H6	0.9300
O2—C1	1.242 (3)	C7—H7	0.9300
O2—Ba1^{vi}	2.727 (2)	C2—Ba1^{vii}	3.199 (3)

O3—C2	1.256 (3)

O3^{i}—Ba1—O2^{ii}	115.43 (7)	N1—Ba1—Ba1^{ix}	132.65 (4)
O3^{i}—Ba1—O1^{iii}	87.17 (7)	C2^{v}—Ba1—Ba1^{ix}	55.55 (4)
O2^{ii}—Ba1—O1^{iii}	150.40 (7)	Ba1^{viii}—Ba1—Ba1^{ix}	107.398 (9)
O3^{i}—Ba1—O1	82.87 (7)	O3^{i}—Ba1—Ba1^{iii}	99.87 (5)
O2^{ii}—Ba1—O1	134.32 (6)	O2^{ii}—Ba1—Ba1^{iii}	142.45 (5)
O1^{iii}—Ba1—O1	63.66 (7)	O1^{iii}—Ba1—Ba1^{iii}	35.23 (4)
O3^{i}—Ba1—O4^{iv}	176.22 (6)	O1—Ba1—Ba1^{iii}	35.07 (4)
O2^{ii}—Ba1—O4^{iv}	68.31 (6)	O4^{iv}—Ba1—Ba1^{iii}	76.62 (4)
O1^{iii}—Ba1—O4^{iv}	89.12 (7)	O4^{v}—Ba1—Ba1^{iii}	121.12 (4)
O1—Ba1—O4^{iv}	94.82 (7)	O3^{v}—Ba1—Ba1^{iii}	97.31 (5)
O3^{i}—Ba1—O4^{v}	69.30 (6)	N1—Ba1—Ba1^{iii}	90.91 (5)
O2^{ii}—Ba1—O4^{v}	84.91 (6)	C2^{v}—Ba1—Ba1^{iii}	107.64 (5)
O1^{iii}—Ba1—O4^{v}	85.89 (6)	Ba1^{viii}—Ba1—Ba1^{iii}	100.719 (6)
O1—Ba1—O4^{v}	139.80 (6)	Ba1^{ix}—Ba1—Ba1^{iii}	100.719 (6)
O4^{iv}—Ba1—O4^{v}	111.18 (5)	C7—N1—C3	117.8 (2)
O3^{i}—Ba1—O3^{v}	111.55 (5)	C7—N1—Ba1	125.67 (17)
O2^{ii}—Ba1—O3^{v}	81.90 (6)	C3—N1—Ba1	116.43 (17)
O1^{iii}—Ba1—O3^{v}	71.64 (6)	C1—O1—Ba1^{iii}	124.82 (18)
O1—Ba1—O3^{v}	132.26 (6)	C1—O1—Ba1	125.07 (18)
O4^{iv}—Ba1—O3^{v}	67.86 (5)	Ba1^{iii}—O1—Ba1	109.69 (7)
O4^{v}—Ba1—O3^{v}	45.65 (6)	C1—O2—Ba1^{vi}	151.01 (19)
O3^{i}—Ba1—N1	76.91 (6)	C2—O3—Ba1^{i}	139.38 (19)
O2^{ii}—Ba1—N1	85.30 (6)	C2—O3—Ba1^{vii}	92.19 (16)
O1^{iii}—Ba1—N1	119.93 (6)	Ba1^{i}—O3—Ba1^{vii}	106.03 (6)
O1—Ba1—N1	57.12 (6)	C2—O4—Ba1^{iv}	119.16 (17)
O4^{iv}—Ba1—N1	104.39 (6)	C2—O4—Ba1^{vii}	94.48 (17)
O4^{v}—Ba1—N1	136.23 (6)	Ba1^{iv}—O4—Ba1^{vii}	105.85 (6)
O3^{v}—Ba1—N1	166.82 (6)	N1—C3—C4	122.0 (3)
O3^{i}—Ba1—C2^{v}	89.14 (6)	N1—C3—C1	117.9 (2)
O2^{ii}—Ba1—C2^{v}	86.19 (6)	C4—C3—C1	120.1 (2)
O1^{iii}—Ba1—C2^{v}	74.73 (7)	C3—C4—C5	119.8 (3)
O1—Ba1—C2^{v}	137.89 (7)	C3—C4—H4	120.1
O4^{iv}—Ba1—C2^{v}	90.59 (6)	C5—C4—H4	120.1
O4^{v}—Ba1—C2^{v}	23.01 (7)	C4—C5—C6	118.3 (2)
O3^{v}—Ba1—C2^{v}	23.11 (6)	C4—C5—C2	120.9 (2)
N1—Ba1—C2^{v}	158.59 (7)	C6—C5—C2	120.8 (3)
O3^{i}—Ba1—Ba1^{viii}	38.44 (4)	C7—C6—C5	118.0 (3)
O2^{ii}—Ba1—Ba1^{viii}	114.66 (4)	C7—C6—H6	121.0
O1^{iii}—Ba1—Ba1^{viii}	70.63 (5)	C5—C6—H6	121.0
O1—Ba1—Ba1^{viii}	105.21 (5)	N1—C7—C6	123.9 (3)
O4^{iv}—Ba1—Ba1^{viii}	140.32 (4)	N1—C7—H7	118.1
O4^{v}—Ba1—Ba1^{viii}	36.42 (4)	C6—C7—H7	118.1
O3^{v}—Ba1—Ba1^{viii}	73.38 (4)	O2—C1—O1	126.1 (3)
N1—Ba1—Ba1^{viii}	115.27 (5)	O2—C1—C3	117.5 (3)
C2^{v}—Ba1—Ba1^{viii}	51.86 (4)	O1—C1—C3	116.4 (2)
O3^{i}—Ba1—Ba1^{ix}	143.17 (4)	O4—C2—O3	125.1 (3)

O2^{ii}—Ba1—Ba1^{ix}	58.04 (5)	O4—C2—C5	117.7 (2)
O1^{iii}—Ba1—Ba1^{ix}	92.37 (5)	O3—C2—C5	117.2 (2)
O1—Ba1—Ba1^{ix}	129.33 (5)	O4—C2—Ba1^{vii}	62.52 (14)
O4^{iv}—Ba1—Ba1^{ix}	37.73 (4)	O3—C2—Ba1^{vii}	64.71 (14)
O4^{v}—Ba1—Ba1^{ix}	73.94 (4)	C5—C2—Ba1^{vii}	162.39 (18)
O3^{v}—Ba1—Ba1^{ix}	35.53 (4)		

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