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catena-Poly[pentaaqua(μ_3-5-carboxylato-2-oxidopyridinium-1-acetato)barium(II)]

Hong Lin[a]* and Yin-Hua He[b]

[a]JinHua Professional-Technical College, Jinhua, Zhejiang 321017, People's Republic of China, and [b]Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China
Correspondence e-mail: jh_ll@126.com

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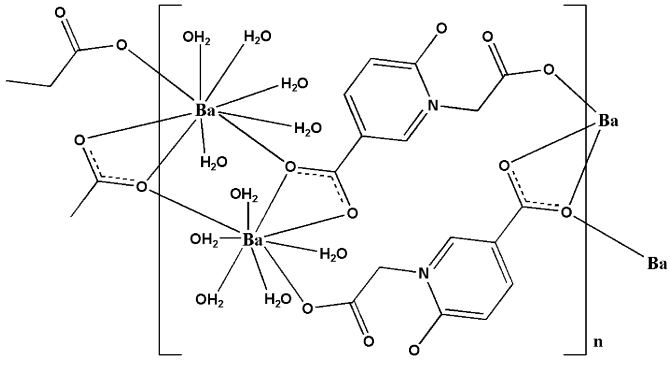
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.016; wR factor = 0.042; data-to-parameter ratio = 14.7.

The title complex, $[Ba(C_8H_5NO_5)(H_2O)_5]_n$, possesses a one-dimensional double-chain structure in which four-membered rings and 18-membered rings are arranged alternately, with the Ba center nine-coordinated by five water molecules and three carboxylate groups from three different ligands. Intermolecular O—H···O hydrogen bonds and strong π–π interactions between pyridine rings extend these chains into a three-dimensional architecture (distance between pairs of adjacent pyridine rings = 3.306 Å; centroid–centroid separation = 3.424 Å).

Related literature

For related literature, see: Chen *et al.* (1998); He & Feng (2007); Shuai *et al.* (2007); Zhang *et al.* (2006).



Experimental

Crystal data

$[Ba(C_8H_5NO_5)(H_2O)_5]$
M_r = 422.55
Triclinic, $P\overline{1}$
a = 7.0051 (14) Å
b = 9.7371 (19) Å
c = 11.201 (2) Å
α = 112.88 (3)°
β = 95.63 (3)°
γ = 100.18 (3)°
V = 681.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.97 mm^{-1}
T = 296 (2) K
0.16 × 0.14 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: empirical (using intensity measurements) (*SADABS*; Sheldrick, 1996)
T_{min} = 0.628, T_{max} = 0.813 (expected range = 0.574–0.743)
11353 measured reflections
3104 independent reflections
2971 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.042
S = 1.01
3104 reflections
211 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ba—O2^{i}	2.7132 (15)	Ba—O1W	2.8560 (17)
Ba—O5W	2.7609 (19)	Ba—O4W	2.856 (2)
Ba—O1	2.7673 (17)	Ba—O3W	2.8593 (19)
Ba—O5^{ii}	2.8129 (19)	Ba—O2	2.976 (2)
Ba—O2W	2.8424 (18)		
O2^{i}—Ba—O5^{ii}	81.75 (5)	O2^{i}—Ba—O4W	139.77 (5)
O1—Ba—O2W	75.98 (6)	O1—Ba—O3W	137.63 (6)
O5W—Ba—O1W	69.51 (6)	O2W—Ba—O3W	144.67 (5)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O5^{iii}	0.855 (16)	2.019 (18)	2.863 (2)	169 (2)
O1W—H1WB···O2W^{iv}	0.844 (16)	1.988 (19)	2.796 (2)	160 (2)
O2W—H2WA···O3^{v}	0.804 (16)	1.897 (16)	2.698 (2)	176 (3)
O2W—H2WB···O1W^{i}	0.826 (16)	2.026 (17)	2.822 (2)	162 (3)
O3W—H3WA···O4^{i}	0.818 (17)	2.015 (18)	2.829 (3)	174 (3)
O3W—H3WB···O4^{iii}	0.852 (17)	2.056 (18)	2.893 (2)	167 (3)
O4W—H4WA···O4W^{vi}	0.787 (16)	2.166 (19)	2.903 (4)	156 (3)
O4W—H4WB···O3^{ii}	0.793 (16)	2.51 (3)	2.992 (3)	120 (2)
O4W—H4WB···O1^{vii}	0.793 (16)	2.608 (19)	3.310 (3)	149 (3)
O5W—H5WA···O1^{vii}	0.831 (17)	1.865 (17)	2.689 (2)	172 (3)
O5W—H5WB···O4^{iii}	0.812 (17)	2.018 (17)	2.823 (3)	171 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2479).

  doi:10.1107/S1600536807058539

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supplementary materials

Acta Cryst. (2007). E**63**, m3204-m3205 [**doi:10.1107/S1600536807058539**]

catena-Poly[pentaaqua(μ_3-5-carboxylato-2-oxidopyridinium-1-acetato)barium(II)]

H. Lin and Y.-H. He

Comment

5-Carboxyl-1-carboxymethyl-2-oxidopyridinium, as a dicarboxylic acid analogue of betaine (He & Feng, 2007), own versatile coordination behavior to metal ions according to the reported complexes, $[Cu(ppbet)_4Cl_2](ClO_4)_2]_n$ (Chen *et al.*, 1998), and $[Cu(4\text{-}OPA)_2]_n$ (Zhang *et al.*, 2006). As illustrated in Fig.1, the title complex has a binuclear structure in which the center Ba^{2+} is nine-coordinated by five water molecules and three carboxylic groups from three different CCOP ligands in monodentate and chelate-bridging bidentate modes, forming a tricapped trigonal prism configuration as [Ba(5—OH-BDC)$(H_2O)_3$] (Shuai *et al.*, 2007). It is interesting that two O atoms of formate groups combine the two Ba^{2+} to form a rhombus while two CCOP ligands adopting the opposite orientations act as bridges to join these rhombuses to be a one-dimensional double chain. It is worth to note intermolecular O—H···O hydrogen bonds are formed to link neighboring chains to form a three-dimensional network. Besides, strong offset face-to-face π-π interactions between pyridinum groups are also involved with the plane-to-plane distance of 3.306 (1) Å and the centroid-centroid distance of 3.424 (3) Å (Fig.2).

Experimental

A solution of $BaCl_2$ (0.2497 g, 1 mmol) and H_2CCOP (0.2025 g, 1 mmol) was mixed and stirred at room temperature. Then the mixture was stood at ambient temperature. By slow evaporation of the solvent, well formed colourless crystals, suitable for X-ray analysis were obtained after two days.

Refinement

The H atoms bonded to C atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 and 0.97 Å, and U_{iso}=1.2U_{eq} (C). The H atoms bonded to O atoms were located in a difference Fourier maps and refined freely.

Figures

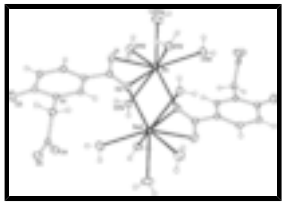

Fig. 1. A view of the molecule of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are shown at the 30% probability level.

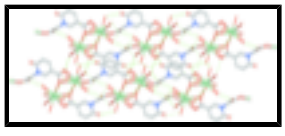

Fig. 2. A view of the three dimensional framework of the title compound. The O—H···O interactions are depicted by dashed lines.

catena-Poly[pentaaqua(μ$_3$-5-carboxylato-2-oxidopyridinium-1-\ acetato)barium(II)]

Crystal data

$[Ba(C_8H_5NO_5)(H_2O)_5]$	$Z = 2$
$M_r = 422.55$	$F_{000} = 412$
Triclinic, $P\overline{1}$	$D_x = 2.061$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.0051$ (14) Å	Cell parameters from 11388 reflections
$b = 9.7371$ (19) Å	$\theta = 2.0$–27.5º
$c = 11.201$ (2) Å	$\mu = 2.97$ mm^{-1}
$\alpha = 112.88$ (3)º	$T = 296$ (2) K
$\beta = 95.63$ (3)º	Block, colourless
$\gamma = 100.18$ (3)º	0.16 × 0.14 × 0.10 mm
$V = 681.0$ (2) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	3104 independent reflections
Radiation source: fine-focus sealed tube	2971 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 296$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.0$º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$h = -9\rightarrow9$
$T_{min} = 0.628$, $T_{max} = 0.813$	$k = -12\rightarrow12$
11353 measured reflections	$l = -14\rightarrow14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.016$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.162P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.003$
3104 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
211 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
15 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Ba	0.600166 (14)	0.757213 (11)	0.602839 (10)	0.02020 (5)
O1	0.4232 (3)	0.72415 (16)	0.35817 (16)	0.0381 (4)
O1W	0.1915 (2)	0.69116 (18)	0.61729 (16)	0.0341 (3)
H1WA	0.134 (4)	0.748 (3)	0.6738 (19)	0.041*
H1WB	0.109 (3)	0.672 (3)	0.5494 (17)	0.041*
O2	0.3509 (2)	0.49709 (16)	0.36455 (14)	0.0304 (3)
O2W	0.8518 (2)	0.62065 (18)	0.43111 (15)	0.0339 (3)
H2WA	0.867 (4)	0.645 (3)	0.371 (2)	0.041*
H2WB	0.825 (4)	0.5260 (19)	0.401 (2)	0.041*
O3	0.0848 (3)	0.28461 (19)	−0.23870 (15)	0.0426 (4)
O3W	0.4998 (3)	0.8244 (2)	0.85769 (16)	0.0448 (4)
H3WA	0.572 (4)	0.856 (3)	0.929 (2)	0.054*
H3WB	0.415 (3)	0.879 (3)	0.871 (3)	0.054*
O4	0.2545 (2)	0.04168 (17)	−0.10934 (15)	0.0330 (3)
O4W	0.8181 (3)	0.9993 (2)	0.5519 (2)	0.0471 (4)
H4WA	0.929 (3)	1.000 (3)	0.545 (3)	0.057*
H4WB	0.805 (4)	1.083 (2)	0.592 (3)	0.057*
O5	−0.0335 (2)	−0.11523 (16)	−0.22398 (15)	0.0321 (3)
O5W	0.4634 (4)	1.0222 (2)	0.6837 (2)	0.0610 (6)
H5WA	0.494 (5)	1.105 (3)	0.677 (3)	0.073*
H5WB	0.404 (5)	1.038 (4)	0.745 (3)	0.073*
N1	0.0942 (2)	0.29402 (17)	−0.03292 (15)	0.0224 (3)
C6	0.3557 (3)	0.5812 (2)	0.30310 (19)	0.0243 (4)
C1	0.1429 (3)	0.3611 (2)	−0.11786 (19)	0.0265 (4)
C7	−0.0354 (3)	0.1403 (2)	−0.0908 (2)	0.0249 (4)
H7A	−0.1350	0.1337	−0.1606	0.030*
H7B	−0.1026	0.1245	−0.0239	0.030*
C4	0.2792 (3)	0.5095 (2)	0.15796 (19)	0.0232 (4)
C2	0.2571 (3)	0.5157 (2)	−0.0563 (2)	0.0276 (4)
H2	0.2876	0.5688	−0.1079	0.033*
C3	0.3217 (3)	0.5864 (2)	0.0757 (2)	0.0265 (4)
H3	0.3953	0.6873	0.1131	0.032*
C8	0.0716 (3)	0.0126 (2)	−0.14697 (18)	0.0227 (4)

C5	0.1647 (3)	0.3642 (2)	0.09955 (18)	0.0227 (4)
H5	0.1336	0.3113	0.1513	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba	0.02295 (7)	0.01711 (6)	0.01811 (7)	0.00351 (4)	0.00071 (4)	0.00599 (5)
O1	0.0590 (10)	0.0203 (7)	0.0255 (7)	−0.0028 (7)	−0.0107 (7)	0.0091 (6)
O1W	0.0306 (8)	0.0331 (8)	0.0303 (8)	0.0070 (6)	0.0020 (6)	0.0055 (7)
O2	0.0442 (8)	0.0217 (7)	0.0233 (7)	0.0038 (6)	−0.0015 (6)	0.0107 (6)
O2W	0.0442 (9)	0.0325 (8)	0.0268 (8)	0.0097 (7)	0.0085 (7)	0.0134 (7)
O3	0.0636 (11)	0.0370 (9)	0.0190 (8)	0.0019 (8)	0.0028 (7)	0.0084 (7)
O3W	0.0505 (10)	0.0552 (11)	0.0252 (8)	0.0262 (9)	0.0016 (7)	0.0084 (8)
O4	0.0271 (7)	0.0337 (8)	0.0299 (8)	0.0104 (6)	−0.0023 (6)	0.0050 (6)
O4W	0.0495 (10)	0.0400 (9)	0.0489 (11)	0.0050 (8)	0.0125 (9)	0.0169 (9)
O5	0.0356 (8)	0.0198 (7)	0.0314 (8)	0.0032 (6)	−0.0006 (6)	0.0037 (6)
O5W	0.0873 (15)	0.0316 (9)	0.0900 (17)	0.0288 (10)	0.0619 (13)	0.0353 (10)
N1	0.0264 (8)	0.0189 (7)	0.0201 (8)	0.0063 (6)	0.0021 (6)	0.0061 (6)
C6	0.0275 (9)	0.0221 (9)	0.0210 (9)	0.0048 (7)	−0.0005 (7)	0.0082 (7)
C1	0.0333 (10)	0.0279 (10)	0.0184 (9)	0.0105 (8)	0.0036 (8)	0.0086 (8)
C7	0.0244 (9)	0.0206 (9)	0.0237 (10)	0.0029 (7)	0.0002 (7)	0.0048 (7)
C4	0.0256 (9)	0.0213 (9)	0.0214 (9)	0.0067 (7)	0.0019 (7)	0.0077 (7)
C2	0.0339 (10)	0.0281 (10)	0.0254 (10)	0.0083 (8)	0.0065 (8)	0.0152 (8)
C3	0.0271 (10)	0.0222 (9)	0.0299 (11)	0.0052 (7)	0.0025 (8)	0.0113 (8)
C8	0.0280 (9)	0.0236 (9)	0.0163 (9)	0.0066 (7)	0.0019 (7)	0.0084 (7)
C5	0.0275 (9)	0.0221 (9)	0.0198 (9)	0.0083 (7)	0.0034 (7)	0.0091 (7)

Geometric parameters (Å, °)

Ba—O2^{i}	2.7132 (15)	O4—C8	1.254 (2)
Ba—O5W	2.7609 (19)	O4W—H4WA	0.787 (16)
Ba—O1	2.7673 (17)	O4W—H4WB	0.793 (16)
Ba—O5^{ii}	2.8129 (19)	O5—C8	1.246 (2)
Ba—O2W	2.8424 (18)	O5—Ba^{iii}	2.8129 (19)
Ba—O1W	2.8560 (17)	O5W—H5WA	0.831 (17)
Ba—O4W	2.856 (2)	O5W—H5WB	0.812 (17)
Ba—O3W	2.8593 (19)	N1—C5	1.364 (2)
Ba—O2	2.976 (2)	N1—C1	1.384 (3)
Ba—C6	3.241 (2)	N1—C7	1.461 (2)
Ba—Ba^{i}	4.5027 (17)	C6—C4	1.494 (3)
O1—C6	1.259 (2)	C1—C2	1.429 (3)
O1W—H1WA	0.855 (16)	C7—C8	1.522 (3)
O1W—H1WB	0.844 (16)	C7—H7A	0.9700
O2—C6	1.256 (2)	C7—H7B	0.9700
O2—Ba^{i}	2.7132 (15)	C4—C5	1.359 (3)
O2W—H2WA	0.804 (16)	C4—C3	1.418 (3)
O2W—H2WB	0.826 (16)	C2—C3	1.354 (3)
O3—C1	1.246 (2)	C2—H2	0.9300

O3W—H3WA	0.818 (17)	C3—H3	0.9300
O3W—H3WB	0.852 (17)	C5—H5	0.9300
O2^{i}—Ba—O5W	149.47 (5)	C6—Ba—Ba^{i}	57.41 (5)
O2^{i}—Ba—O1	118.73 (5)	C6—O1—Ba	100.42 (12)
O5W—Ba—O1	81.72 (7)	Ba—O1W—H1WA	126.3 (17)
O2^{i}—Ba—O5^{ii}	81.75 (5)	Ba—O1W—H1WB	117.4 (17)
O5W—Ba—O5^{ii}	96.55 (7)	H1WA—O1W—H1WB	97.3 (19)
O1—Ba—O5^{ii}	140.28 (5)	C6—O2—Ba^{i}	153.83 (13)
O2^{i}—Ba—O2W	71.99 (5)	C6—O2—Ba	90.53 (11)
O5W—Ba—O2W	137.98 (5)	Ba^{i}—O2—Ba	104.56 (5)
O1—Ba—O2W	75.98 (6)	Ba—O2W—H2WA	118.5 (19)
O5^{ii}—Ba—O2W	79.65 (5)	Ba—O2W—H2WB	114.0 (19)
O2^{i}—Ba—O1W	91.48 (5)	H2WA—O2W—H2WB	107 (2)
O5W—Ba—O1W	69.51 (6)	Ba—O3W—H3WA	129 (2)
O1—Ba—O1W	78.36 (6)	Ba—O3W—H3WB	111 (2)
O5^{ii}—Ba—O1W	138.31 (5)	H3WA—O3W—H3WB	104 (2)
O2W—Ba—O1W	137.03 (5)	Ba—O4W—H4WA	118 (2)
O2^{i}—Ba—O4W	139.77 (5)	Ba—O4W—H4WB	118 (2)
O5W—Ba—O4W	64.80 (6)	H4WA—O4W—H4WB	111 (2)
O1—Ba—O4W	73.10 (6)	C8—O5—Ba^{iii}	139.64 (13)
O5^{ii}—Ba—O4W	70.48 (6)	Ba—O5W—H5WA	135 (2)
O2W—Ba—O4W	74.76 (6)	Ba—O5W—H5WB	116 (2)
O1W—Ba—O4W	128.59 (6)	H5WA—O5W—H5WB	106 (2)
O2^{i}—Ba—O3W	79.46 (6)	C5—N1—C1	122.79 (16)
O5W—Ba—O3W	70.65 (6)	C5—N1—C7	119.92 (16)
O1—Ba—O3W	137.63 (6)	C1—N1—C7	117.28 (16)
O5^{ii}—Ba—O3W	76.00 (6)	O2—C6—O1	122.98 (18)
O2W—Ba—O3W	144.67 (5)	O2—C6—C4	119.01 (17)
O1W—Ba—O3W	62.34 (6)	O1—C6—C4	118.01 (17)
O4W—Ba—O3W	119.19 (6)	O2—C6—Ba	66.66 (10)
O2^{i}—Ba—O2	75.44 (5)	O1—C6—Ba	57.12 (11)
O5W—Ba—O2	114.74 (7)	C4—C6—Ba	169.13 (13)
O1—Ba—O2	45.08 (4)	O3—C1—N1	118.76 (18)
O5^{ii}—Ba—O2	147.62 (5)	O3—C1—C2	125.75 (19)
O2W—Ba—O2	71.66 (5)	N1—C1—C2	115.48 (17)
O1W—Ba—O2	65.78 (5)	N1—C7—C8	113.86 (16)
O4W—Ba—O2	114.43 (5)	N1—C7—H7A	108.8
O3W—Ba—O2	120.87 (6)	C8—C7—H7A	108.8
O2^{i}—Ba—C6	96.73 (5)	N1—C7—H7B	108.8
O5W—Ba—C6	99.81 (7)	C8—C7—H7B	108.8
O1—Ba—C6	22.46 (4)	H7A—C7—H7B	107.7
O5^{ii}—Ba—C6	148.80 (5)	C5—C4—C3	117.30 (18)
O2W—Ba—C6	70.40 (5)	C5—C4—C6	119.97 (18)
O1W—Ba—C6	72.70 (6)	C3—C4—C6	122.73 (17)
O4W—Ba—C6	92.84 (6)	C3—C2—C1	121.25 (18)

O3W—Ba—C6	134.65 (6)	C3—C2—H2	119.4
O2—Ba—C6	22.81 (4)	C1—C2—H2	119.4
O2^{i}—Ba—Ba^{i}	39.76 (3)	C2—C3—C4	121.21 (18)
O5W—Ba—Ba^{i}	142.72 (5)	C2—C3—H3	119.4
O1—Ba—Ba^{i}	79.81 (5)	C4—C3—H3	119.4
O5^{ii}—Ba—Ba^{i}	118.14 (4)	O5—C8—O4	125.32 (19)
O2W—Ba—Ba^{i}	66.78 (4)	O5—C8—C7	116.23 (17)
O1W—Ba—Ba^{i}	75.19 (5)	O4—C8—C7	118.40 (17)
O4W—Ba—Ba^{i}	137.17 (4)	C4—C5—N1	121.72 (18)
O3W—Ba—Ba^{i}	103.23 (5)	C4—C5—H5	119.1
O2—Ba—Ba^{i}	35.68 (3)	N1—C5—H5	119.1
O2^{i}—Ba—O1—C6	12.49 (15)	O5W—Ba—C6—O1	36.77 (14)
O5W—Ba—O1—C6	−143.41 (14)	O5^{ii}—Ba—C6—O1	−83.81 (16)
O5^{ii}—Ba—O1—C6	126.30 (13)	O2W—Ba—C6—O1	−100.86 (14)
O2W—Ba—O1—C6	72.47 (14)	O1W—Ba—C6—O1	101.56 (14)
O1W—Ba—O1—C6	−72.75 (14)	O4W—Ba—C6—O1	−28.14 (14)
O4W—Ba—O1—C6	150.51 (15)	O3W—Ba—C6—O1	109.20 (15)
O3W—Ba—O1—C6	−94.44 (15)	O2—Ba—C6—O1	170.0 (2)
O2—Ba—O1—C6	−5.47 (12)	Ba^{i}—Ba—C6—O1	−175.26 (15)
Ba^{i}—Ba—O1—C6	4.06 (13)	O2^{i}—Ba—C6—C4	−102.6 (7)
O2^{i}—Ba—O2—C6	−158.39 (15)	O5W—Ba—C6—C4	103.2 (7)
O5W—Ba—O2—C6	52.26 (13)	O1—Ba—C6—C4	66.4 (7)
O1—Ba—O2—C6	5.39 (12)	O5^{ii}—Ba—C6—C4	−17.4 (7)
O5^{ii}—Ba—O2—C6	−111.73 (13)	O2W—Ba—C6—C4	−34.5 (7)
O2W—Ba—O2—C6	−82.90 (12)	O1W—Ba—C6—C4	167.9 (7)
O1W—Ba—O2—C6	103.21 (13)	O4W—Ba—C6—C4	38.3 (7)
O4W—Ba—O2—C6	−19.94 (13)	O3W—Ba—C6—C4	175.6 (7)
O3W—Ba—O2—C6	133.67 (12)	O2—Ba—C6—C4	−123.6 (7)
Ba^{i}—Ba—O2—C6	−158.39 (15)	Ba^{i}—Ba—C6—C4	−108.9 (7)
O2^{i}—Ba—O2—Ba^{i}	0.0	C5—N1—C1—O3	174.46 (19)
O5W—Ba—O2—Ba^{i}	−149.35 (5)	C7—N1—C1—O3	−4.3 (3)
O1—Ba—O2—Ba^{i}	163.78 (9)	C5—N1—C1—C2	−5.9 (3)
O5^{ii}—Ba—O2—Ba^{i}	46.66 (10)	C7—N1—C1—C2	175.29 (17)
O2W—Ba—O2—Ba^{i}	75.49 (6)	C5—N1—C7—C8	−95.9 (2)
O1W—Ba—O2—Ba^{i}	−98.40 (6)	C1—N1—C7—C8	82.9 (2)
O4W—Ba—O2—Ba^{i}	138.45 (6)	O2—C6—C4—C5	15.6 (3)
O3W—Ba—O2—Ba^{i}	−67.94 (7)	O1—C6—C4—C5	−164.69 (19)
C6—Ba—O2—Ba^{i}	158.39 (15)	Ba—C6—C4—C5	134.7 (6)
Ba^{i}—O2—C6—O1	−136.1 (2)	O2—C6—C4—C3	−164.05 (19)
Ba—O2—C6—O1	−10.0 (2)	O1—C6—C4—C3	15.7 (3)
Ba^{i}—O2—C6—C4	43.6 (4)	Ba—C6—C4—C3	−45.0 (8)
Ba—O2—C6—C4	169.66 (16)	O3—C1—C2—C3	−176.6 (2)
Ba^{i}—O2—C6—Ba	−126.1 (3)	N1—C1—C2—C3	3.8 (3)

Ba—O1—C6—O2	11.0 (2)	C1—C2—C3—C4	0.3 (3)
Ba—O1—C6—C4	−168.71 (15)	C5—C4—C3—C2	−2.5 (3)
$O2^{i}$—Ba—C6—O2	21.03 (14)	C6—C4—C3—C2	177.12 (19)
O5W—Ba—C6—O2	−133.21 (12)	Ba^{iii}—O5—C8—O4	−157.84 (15)
O1—Ba—C6—O2	−170.0 (2)	Ba^{iii}—O5—C8—C7	24.9 (3)
$O5^{ii}$—Ba—C6—O2	106.21 (13)	N1—C7—C8—O5	−163.47 (17)
O2W—Ba—C6—O2	89.16 (12)	N1—C7—C8—O4	19.0 (3)
O1W—Ba—C6—O2	−68.42 (12)	C3—C4—C5—N1	0.5 (3)
O4W—Ba—C6—O2	161.88 (12)	C6—C4—C5—N1	−179.13 (17)
O3W—Ba—C6—O2	−60.78 (14)	C1—N1—C5—C4	3.9 (3)
Ba^{i}—Ba—C6—O2	14.77 (10)	C7—N1—C5—C4	−177.34 (18)
$O2^{i}$—Ba—C6—O1	−168.99 (14)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···$O5^{iv}$	0.855 (16)	2.019 (18)	2.863 (2)	169 (2)
O1W—H1WB···$O2W^{v}$	0.844 (16)	1.988 (19)	2.796 (2)	160 (2)
O2W—H2WA···$O3^{vi}$	0.804 (16)	1.897 (16)	2.698 (2)	176 (3)
O2W—H2WB···$O1W^{i}$	0.826 (16)	2.026 (17)	2.822 (2)	162 (3)
O3W—H3WA···$O4^{i}$	0.818 (17)	2.015 (18)	2.829 (3)	174 (3)
O3W—H3WB···$O4^{iv}$	0.852 (17)	2.056 (18)	2.893 (2)	167 (3)
O4W—H4WA···$O4W^{vii}$	0.787 (16)	2.166 (19)	2.903 (4)	156 (3)
O4W—H4WB···$O3^{ii}$	0.793 (16)	2.51 (3)	2.992 (3)	120 (2)
O4W—H4WB···$O1^{viii}$	0.793 (16)	2.608 (19)	3.310 (3)	149 (3)
O5W—H5WA···$O1^{viii}$	0.831 (17)	1.865 (17)	2.689 (2)	172 (3)
O5W—H5WB···$O4^{iv}$	0.812 (17)	2.018 (17)	2.823 (3)	171 (3)

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

Fig. 1

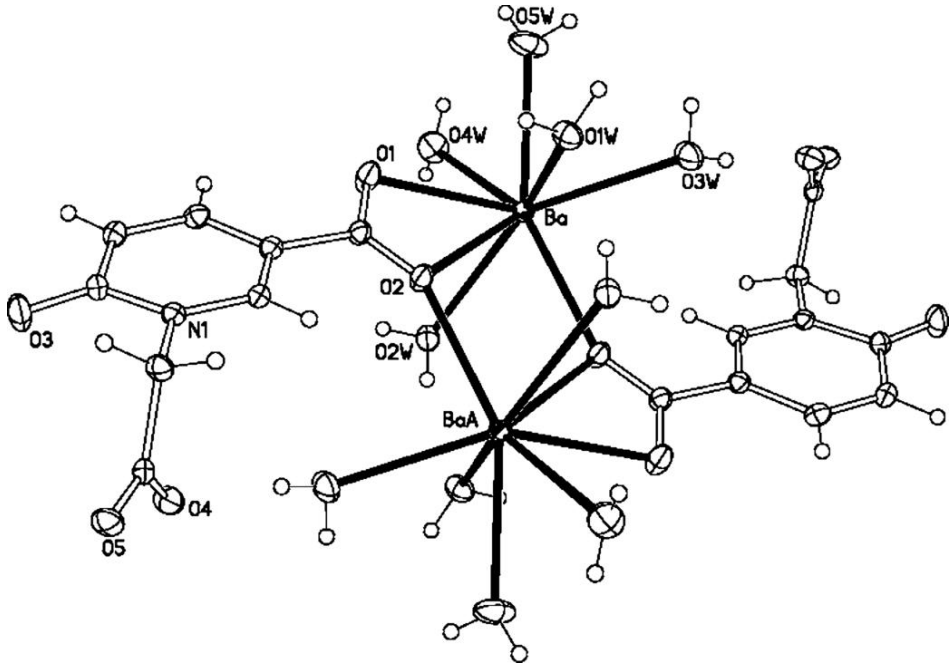

Fig. 2