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Poly[[μ_2-aqua-aqua(μ_3-3,5-dinitrosalicylato)barium(II)] monohydrate]

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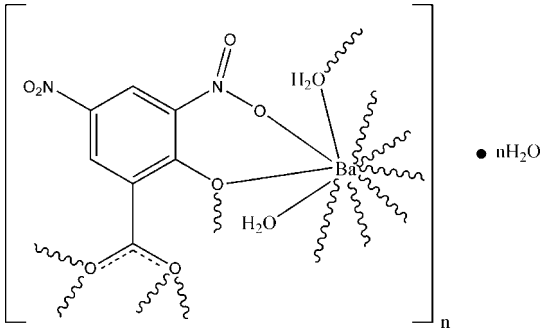
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.068; data-to-parameter ratio = 11.9.

In the title coordination polymer, $\{[Ba(C_7H_2N_2O_7)(H_2O)_2]\cdot H_2O\}_n$, the Ba^{II} atom is ten-coordinated by seven O atoms from four 3,5-dinitrosalicylatate ligands, two μ_2-bridging aqua ligands and one water molecule. The coordination mode is best described as a bicapped square-antiprismatic geometry. The 3,5-dinitrosalicylatate ligands bridge three Ba atoms. Centrosymmetrically related dinuclear barium units, with a Ba···Ba separation of 4.767 (5) Å, form infinite chains, which are further self-assembled into a supramolecular network through intermolecular O—H···O hydrogen-bonding interactions between O atoms of 3,5-dinitrosalicylatate ligands and water molecules.

Related literature

For related literature, see: Song *et al.* (2007).



Experimental

Crystal data

$[Ba(C_7H_2N_2O_7)(H_2O)_2]\cdot H_2O$
M_r = 417.49
Monoclinic, $P2_1/c$
a = 11.9649 (6) Å
b = 4.1866 (2) Å
c = 26.121 (1) Å
β = 109.332 (3)°
V = 1234.7 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.27 mm^{-1}
T = 296 (2) K
0.30 × 0.26 × 0.23 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.392, T_{max} = 0.471
8615 measured reflections
2374 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.05
2374 reflections
199 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3W—H6W···O7^{i}	0.82 (3)	2.27 (3)	2.916 (4)	135 (4)
O3W—H5W···O5^{ii}	0.82 (4)	2.60 (4)	2.985 (4)	110 (3)
O3W—H5W···O2W^{iii}	0.82 (4)	2.04 (3)	2.755 (4)	145 (4)
O2W—H4W···N1^{iv}	0.83 (3)	2.69 (4)	3.340 (4)	137 (4)
O2W—H4W···O4^{iv}	0.83 (3)	2.55 (4)	3.080 (4)	123 (3)
O2W—H4W···O5^{iv}	0.83 (3)	2.25 (3)	2.993 (4)	150 (5)
O2W—H3W···O3^{v}	0.83 (3)	2.01 (2)	2.730 (4)	145 (4)
O1W—H1W···O3W^{v}	0.83 (3)	1.991 (16)	2.798 (4)	164 (4)
O1W—H2W···O3W^{vi}	0.83 (3)	1.90 (3)	2.725 (4)	171 (4)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *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: IM2052).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supplementary materials

Acta Cryst. (2008). E**64**, m551 [**doi:10.1107/S1600536808006338**]

Poly[[μ_2-aqua-aqua(μ_3-3,5-dinitrosalicylato)barium(II)] monohydrate]

W.-D. Song, R.-Z. Fan, C.-S. Gu and X.-M. Hao

Comment

In the structural investigation of 3,5-dinitrosalicylatato complexes, it has been found that the 3,5-dinitrosalicylatato moiety functions as a multidentate ligand (Song *et al.*, 2007) with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Ba complex obtained by the reaction of 3,5-dinitrosalicylic acid and barium chloride in alkaline aqueous solution.

As illustrated in Figure 1, the Ba^{II} atom displays a bicapped square antiprismatic coordination environment, defined by seven O atoms from four 3,5-dinitrosalicylatato ligands, two μ_2-bridging aqua ligands and one water molecule. The 3,5-dinitrosalicylatato ligands link barium ions to form infinite chains, which are further self-assembled into a supramolecular network through intermolecular O—H···O hydrogen bonding interactions (Table 1) involving the uncoordinating water molecules, coordinating water molecules as donors and O atoms of 3,5-dinitrosalicylatato ligands as acceptors (Fig. 2).

Experimental

A mixture of barium chloride (1 mmol), 3,5-dinitrosalicylic acid (1 mmol), NaOH (1.5 mmol) and H_2O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The obtained crystals obtained were washed with water and dryed in air.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.84 Å and H···H = 1.39 Å, each within a standard deviation of 0.01 Å, and with U_{iso}(H) = 1.5 U_{eq}(O)

Figures

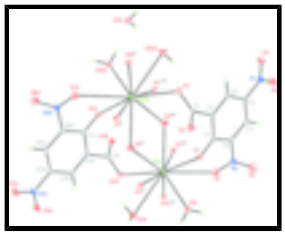


Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids.

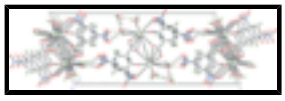


Fig. 2. A packing view of the title compound. The intermolecluar hydrogen bonds are shown as dashed lines.

Poly[[μ_2-aqua-aqua(μ_3-3,5-dinitrosalicylato)barium(II)] monohydrate]

Crystal data

$[Ba(C_7H_2N_2O_7)(H_2O)_2]\cdot H_2O$	$F_{000} = 800$
$M_r = 417.49$	$D_x = 2.246$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5837 reflections
$a = 11.9649$ (6) Å	$\theta = 2.8$–27.9º
$b = 4.1866$ (2) Å	$\mu = 3.27$ mm^{-1}
$c = 26.121$ (1) Å	$T = 296$ (2) K
$\beta = 109.332$ (3)º	Block, yellow
$V = 1234.7$ (1) Å^3	0.30 × 0.26 × 0.23 mm
$Z = 4$	

Data collection

Bruker APEXII area-detector diffractometer	2374 independent reflections
Radiation source: fine-focus sealed tube	2189 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 296$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14\rightarrow14$
$T_{min} = 0.392$, $T_{max} = 0.472$	$k = -4\rightarrow4$
8615 measured reflections	$l = -31\rightarrow32$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 1.4739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
2374 reflections	$\Delta\rho_{max} = 1.03$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -1.30$ e Å^{-3}
9 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.698106 (16)	0.59849 (4)	0.002749 (8)	0.01250 (10)
O1	0.7177 (2)	0.1028 (5)	0.06998 (10)	0.0150 (5)
O2	0.5320 (2)	−0.3574 (6)	0.05297 (11)	0.0211 (6)
O3	0.4012 (2)	−0.0694 (6)	0.07602 (11)	0.0190 (6)
O4	0.5934 (3)	0.0066 (8)	0.28282 (12)	0.0311 (7)
O5	0.7491 (3)	0.3054 (8)	0.31157 (12)	0.0359 (7)
O6	0.9954 (3)	0.3764 (8)	0.19294 (14)	0.0416 (9)
O7	0.8915 (2)	0.5460 (7)	0.11347 (12)	0.0251 (6)
N1	0.6755 (3)	0.1544 (8)	0.27501 (14)	0.0245 (7)
N2	0.9007 (3)	0.4015 (7)	0.15565 (14)	0.0205 (7)
C1	0.5067 (3)	−0.1530 (8)	0.08248 (14)	0.0116 (7)
C2	0.6052 (3)	−0.0051 (9)	0.12815 (14)	0.0129 (7)
C3	0.5950 (3)	0.0128 (9)	0.17862 (15)	0.0167 (7)
H3	0.5270	−0.0629	0.1844	0.020*
C4	0.6874 (3)	0.1461 (9)	0.22201 (15)	0.0178 (8)
C5	0.7878 (3)	0.2691 (9)	0.21433 (15)	0.0191 (8)
H5	0.8488	0.3552	0.2431	0.023*
C6	0.7951 (3)	0.2603 (9)	0.16271 (14)	0.0158 (7)
C7	0.7074 (3)	0.1200 (8)	0.11687 (15)	0.0146 (8)
O1W	0.8608 (2)	0.1295 (6)	0.00092 (12)	0.0205 (6)
H2W	0.922 (2)	0.101 (10)	0.0272 (9)	0.031*
H1W	0.881 (3)	0.137 (10)	−0.0265 (9)	0.031*
O2W	0.7483 (2)	0.6467 (6)	−0.09980 (12)	0.0223 (6)
H3W	0.688 (2)	0.758 (8)	−0.1068 (17)	0.033*
H4W	0.732 (3)	0.484 (6)	−0.1189 (16)	0.033*
O3W	0.0565 (2)	0.9715 (8)	0.08622 (12)	0.0255 (6)
H5W	0.110 (3)	1.093 (8)	0.1033 (15)	0.038*
H6W	0.047 (4)	0.837 (8)	0.1074 (13)	0.038*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Ba1	0.01402 (13)	0.01055 (14)	0.01455 (15)	−0.00009 (7)	0.00690 (10)	−0.00038 (8)
O1	0.0191 (13)	0.0156 (14)	0.0133 (13)	−0.0010 (9)	0.0091 (11)	−0.0007 (10)
O2	0.0199 (13)	0.0222 (15)	0.0235 (15)	−0.0031 (10)	0.0105 (12)	−0.0089 (11)
O3	0.0142 (12)	0.0185 (15)	0.0238 (15)	0.0005 (10)	0.0055 (11)	−0.0015 (11)
O4	0.0331 (16)	0.0413 (17)	0.0244 (16)	−0.0037 (14)	0.0167 (13)	0.0019 (15)
O5	0.0411 (18)	0.0464 (19)	0.0186 (16)	−0.0102 (15)	0.0077 (14)	−0.0100 (15)
O6	0.0227 (16)	0.066 (3)	0.033 (2)	−0.0138 (14)	0.0056 (15)	0.0021 (16)
O7	0.0248 (14)	0.0226 (15)	0.0300 (17)	−0.0044 (11)	0.0117 (12)	0.0052 (13)
N1	0.0296 (18)	0.0263 (18)	0.0184 (18)	0.0037 (14)	0.0089 (15)	−0.0003 (14)
N2	0.0151 (15)	0.0223 (19)	0.0230 (19)	−0.0046 (12)	0.0049 (14)	−0.0040 (14)
C1	0.0132 (16)	0.0130 (18)	0.0082 (17)	−0.0010 (13)	0.0030 (14)	0.0023 (13)
C2	0.0163 (16)	0.0102 (17)	0.0128 (18)	0.0025 (14)	0.0056 (14)	0.0018 (14)
C3	0.0178 (17)	0.0153 (18)	0.0178 (19)	0.0006 (15)	0.0071 (15)	0.0015 (16)
C4	0.0214 (18)	0.021 (2)	0.0116 (18)	0.0022 (14)	0.0060 (15)	−0.0015 (15)
C5	0.0190 (17)	0.018 (2)	0.0166 (19)	−0.0003 (15)	0.0013 (15)	−0.0030 (16)
C6	0.0129 (16)	0.016 (2)	0.0181 (19)	−0.0012 (14)	0.0042 (14)	−0.0002 (15)
C7	0.0184 (18)	0.0121 (19)	0.0146 (19)	0.0044 (13)	0.0074 (15)	0.0040 (13)
O1W	0.0156 (13)	0.0291 (16)	0.0186 (15)	0.0036 (10)	0.0079 (11)	0.0005 (12)
O2W	0.0290 (15)	0.0188 (15)	0.0222 (15)	0.0010 (11)	0.0126 (13)	−0.0019 (11)
O3W	0.0206 (14)	0.0334 (17)	0.0235 (16)	−0.0020 (12)	0.0086 (12)	0.0046 (13)

Geometric parameters (Å, °)

Ba1—O1	2.678 (2)	O5—N1	1.237 (4)
Ba1—O1^{i}	2.706 (2)	O6—N2	1.230 (5)
Ba1—O2^{i}	2.726 (3)	O7—N2	1.230 (4)
Ba1—O1W	2.777 (3)	N1—C4	1.438 (5)
Ba1—O3^{ii}	2.813 (3)	N2—C6	1.462 (4)
Ba1—O2^{iii}	2.840 (3)	C1—C2	1.505 (5)
Ba1—O2W	2.940 (3)	C1—Ba1^{iii}	3.290 (3)
Ba1—O1W^{i}	2.966 (3)	C2—C3	1.366 (5)
Ba1—O3^{iii}	2.989 (3)	C2—C7	1.447 (5)
Ba1—O7	3.056 (3)	C3—C4	1.410 (5)
Ba1—C1^{iii}	3.290 (3)	C3—H3	0.9300
Ba1—Ba1^{i}	4.18660 (19)	C4—C5	1.382 (5)
Ba1—H3W	2.90 (5)	C5—C6	1.380 (5)
O1—C7	1.273 (4)	C5—H5	0.9300
O1—Ba1^{iv}	2.706 (2)	C6—C7	1.431 (5)
O2—C1	1.254 (4)	O1W—Ba1^{iv}	2.966 (3)
O2—Ba1^{iv}	2.726 (3)	O1W—H2W	0.83 (4)
O2—Ba1^{iii}	2.840 (3)	O1W—H1W	0.83 (4)
O3—C1	1.266 (4)	O2W—H3W	0.83 (4)
O3—Ba1^{ii}	2.813 (3)	O2W—H4W	0.83 (4)
O3—Ba1^{iii}	2.989 (3)	O3W—H5W	0.82 (4)
O4—N1	1.233 (4)	O3W—H6W	0.83 (4)
O1—Ba1—O1^{i}	102.07 (8)	O7—Ba1—Ba1^{i}	94.12 (5)

O1—Ba1—O2^{i}	69.92 (8)	C1^{iii}—Ba1—Ba1^{i}	124.53 (6)
O1^{i}—Ba1—O2^{i}	63.59 (7)	O1—Ba1—H3W	142.3 (6)
O1—Ba1—O1W	63.49 (7)	O1^{i}—Ba1—H3W	115.3 (6)
O1^{i}—Ba1—O1W	130.70 (8)	O2^{i}—Ba1—H3W	131.3 (3)
O2^{i}—Ba1—O1W	133.10 (8)	O1W—Ba1—H3W	86.9 (3)
O1—Ba1—O3^{ii}	161.23 (8)	O3^{ii}—Ba1—H3W	41.2 (3)
O1^{i}—Ba1—O3^{ii}	81.53 (7)	O2^{iii}—Ba1—H3W	81.9 (7)
O2^{i}—Ba1—O3^{ii}	96.08 (8)	O2W—Ba1—H3W	16.3 (6)
O1W—Ba1—O3^{ii}	127.72 (8)	O1W^{i}—Ba1—H3W	68.0 (7)
O1—Ba1—O2^{iii}	85.43 (8)	O3^{iii}—Ba1—H3W	67.3 (7)
O1^{i}—Ba1—O2^{iii}	118.10 (7)	O7—Ba1—H3W	136.2 (6)
O2^{i}—Ba1—O2^{iii}	62.17 (9)	C1^{iii}—Ba1—H3W	71.6 (7)
O1W—Ba1—O2^{iii}	107.83 (7)	Ba1^{i}—Ba1—H3W	76.7 (6)
O3^{ii}—Ba1—O2^{iii}	76.78 (8)	C7—O1—Ba1	124.9 (2)
O1—Ba1—O2W	130.60 (7)	C7—O1—Ba1^{iv}	130.8 (2)
O1^{i}—Ba1—O2W	122.52 (7)	Ba1—O1—Ba1^{iv}	102.07 (8)
O2^{i}—Ba1—O2W	146.64 (8)	C1—O2—Ba1^{iv}	134.8 (2)
O1W—Ba1—O2W	71.15 (8)	C1—O2—Ba1^{iii}	99.6 (2)
O3^{ii}—Ba1—O2W	56.60 (7)	Ba1^{iv}—O2—Ba1^{iii}	117.83 (9)
O2^{iii}—Ba1—O2W	90.76 (8)	C1—O3—Ba1^{ii}	116.9 (2)
O1—Ba1—O1W^{i}	132.52 (7)	C1—O3—Ba1^{iii}	92.2 (2)
O1^{i}—Ba1—O1W^{i}	60.61 (7)	Ba1^{ii}—O3—Ba1^{iii}	92.33 (8)
O2^{i}—Ba1—O1W^{i}	122.95 (7)	N2—O7—Ba1	134.3 (2)
O1W—Ba1—O1W^{i}	93.55 (7)	O4—N1—O5	122.1 (3)
O3^{ii}—Ba1—O1W^{i}	65.38 (7)	O4—N1—C4	119.0 (3)
O2^{iii}—Ba1—O1W^{i}	142.04 (8)	O5—N1—C4	118.9 (3)
O2W—Ba1—O1W^{i}	66.46 (8)	O7—N2—O6	122.5 (3)
O1—Ba1—O3^{iii}	78.80 (7)	O7—N2—C6	119.2 (3)
O1^{i}—Ba1—O3^{iii}	162.60 (7)	O6—N2—C6	118.3 (3)
O2^{i}—Ba1—O3^{iii}	101.22 (7)	O2—C1—O3	122.7 (3)
O1W—Ba1—O3^{iii}	65.50 (7)	O2—C1—C2	118.9 (3)
O3^{ii}—Ba1—O3^{iii}	92.33 (8)	O3—C1—C2	118.5 (3)
O2^{iii}—Ba1—O3^{iii}	44.50 (7)	O2—C1—Ba1^{iii}	58.32 (18)
O2W—Ba1—O3^{iii}	65.05 (7)	O3—C1—Ba1^{iii}	65.18 (18)
O1W^{i}—Ba1—O3^{iii}	131.14 (7)	C2—C1—Ba1^{iii}	169.1 (2)
O1—Ba1—O7	56.58 (7)	C3—C2—C7	121.9 (3)
O1^{i}—Ba1—O7	64.28 (8)	C3—C2—C1	119.4 (3)
O2^{i}—Ba1—O7	89.64 (8)	C7—C2—C1	118.7 (3)
O1W—Ba1—O7	69.50 (8)	C2—C3—C4	120.0 (3)
O3^{ii}—Ba1—O7	138.31 (7)	C2—C3—H3	120.0
O2^{iii}—Ba1—O7	139.60 (8)	C4—C3—H3	120.0

O2W—Ba1—O7	123.25 (7)	C5—C4—C3	121.3 (3)
O1W^{i}—Ba1—O7	76.92 (7)	C5—C4—N1	119.9 (3)
O3^{iii}—Ba1—O7	127.03 (7)	C3—C4—N1	118.8 (3)
O1—Ba1—C1^{iii}	83.60 (8)	C6—C5—C4	118.1 (3)
O1^{i}—Ba1—C1^{iii}	140.04 (8)	C6—C5—H5	121.0
O2^{i}—Ba1—C1^{iii}	82.29 (8)	C4—C5—H5	121.0
O1W—Ba1—C1^{iii}	87.53 (8)	C5—C6—C7	124.2 (3)
O3^{ii}—Ba1—C1^{iii}	82.12 (8)	C5—C6—N2	116.7 (3)
O2^{iii}—Ba1—C1^{iii}	22.07 (8)	C7—C6—N2	119.1 (3)
O2W—Ba1—C1^{iii}	75.72 (8)	O1—C7—C6	123.4 (3)
O1W^{i}—Ba1—C1^{iii}	139.44 (8)	O1—C7—C2	122.2 (3)
O3^{iii}—Ba1—C1^{iii}	22.61 (8)	C6—C7—C2	114.4 (3)
O7—Ba1—C1^{iii}	139.53 (8)	Ba1—O1W—Ba1^{iv}	93.55 (7)
O1—Ba1—Ba1^{i}	140.79 (5)	Ba1—O1W—H2W	121 (3)
O1^{i}—Ba1—Ba1^{i}	38.72 (5)	Ba1^{iv}—O1W—H2W	107 (3)
O2^{i}—Ba1—Ba1^{i}	86.11 (5)	Ba1—O1W—H1W	113 (3)
O1W—Ba1—Ba1^{i}	135.00 (5)	Ba1^{iv}—O1W—H1W	115 (3)
O3^{ii}—Ba1—Ba1^{i}	45.50 (5)	H2W—O1W—H1W	106.4 (17)
O2^{iii}—Ba1—Ba1^{i}	110.82 (5)	Ba1—O2W—H3W	79 (3)
O2W—Ba1—Ba1^{i}	86.06 (5)	Ba1—O2W—H4W	114 (4)
O1W^{i}—Ba1—Ba1^{i}	41.45 (5)	H3W—O2W—H4W	108 (4)
O3^{iii}—Ba1—Ba1^{i}	137.83 (5)	H5W—O3W—H6W	108 (4)

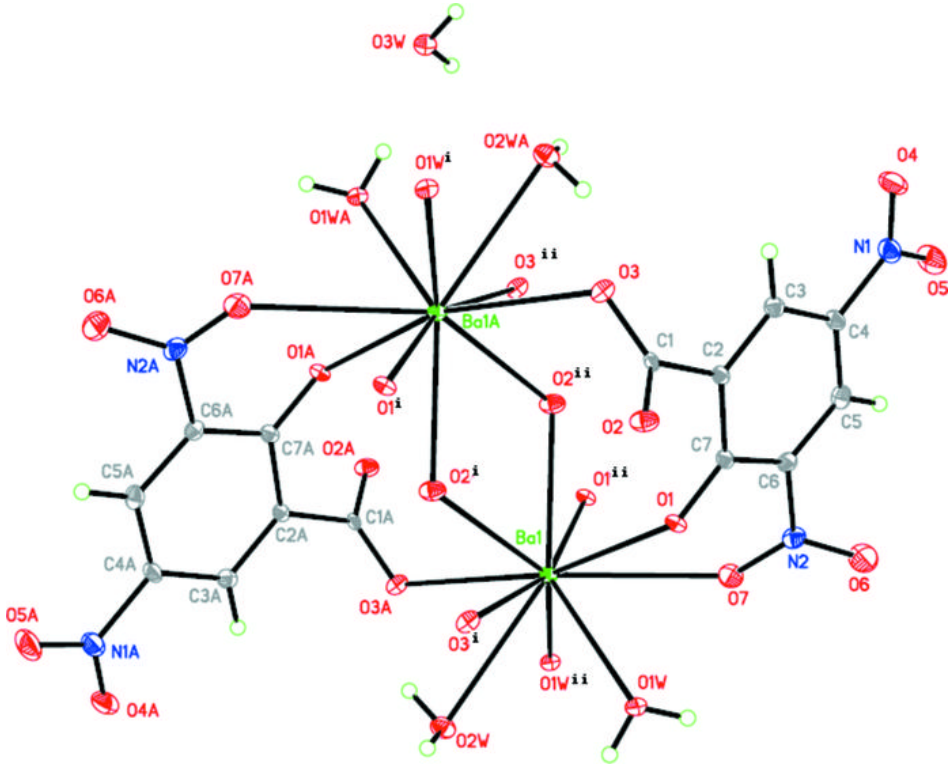
Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*, −*z*; (iv) *x*, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H6W···O7^{v}	0.82 (3)	2.27 (3)	2.916 (4)	135 (4)
O3W—H5W···O5^{vi}	0.82 (4)	2.60 (4)	2.985 (4)	110 (3)
O3W—H5W···O2W^{vii}	0.82 (4)	2.04 (3)	2.755 (4)	145 (4)
O2W—H4W···N1^{viii}	0.83 (3)	2.69 (4)	3.340 (4)	137 (4)
O2W—H4W···O4^{viii}	0.83 (3)	2.55 (4)	3.080 (4)	123 (3)
O2W—H4W···O5^{viii}	0.83 (3)	2.25 (3)	2.993 (4)	150 (5)
O2W—H3W···O3^{ii}	0.83 (3)	2.01 (2)	2.730 (4)	145 (4)
O1W—H1W···O3W^{ii}	0.83 (3)	1.991 (16)	2.798 (4)	164 (4)
O1W—H2W···O3W^{ix}	0.83 (3)	1.90 (3)	2.725 (4)	171 (4)

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

Fig. 1


O3W
O2WA
O1W^{i}
O1WA
O4
N1
O5
O3^{ii}
O3
O7A
C3
O6A
Ba1A
C4
N2A
O1A
C1
C2
O1^{i}
O2^{ii}
O2
C5
C6A
C7A
O2A
C7
C5A
O2^{i}
O1^{ii}
C6
O1
C1A
C2A
Ba1
N2
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O5A
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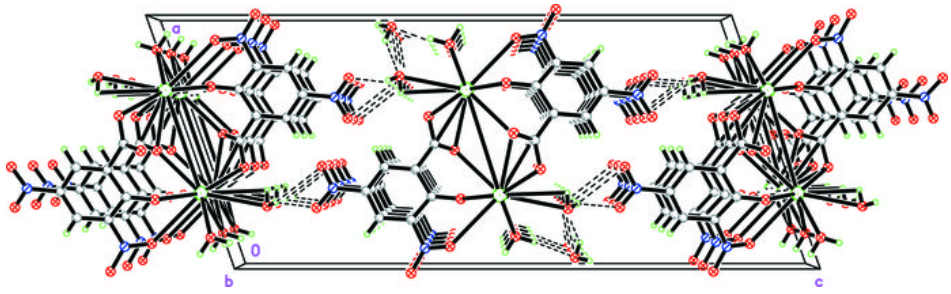
Fig. 2