Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

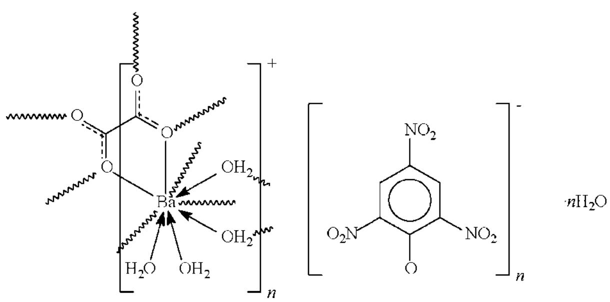
Poly[[tetra-μ_2-aqua-diaqua-μ_6-oxalato-barium(II)] 2,4,6-trinitrophenolate monohydrate]. Corrigendum

Peng-Zhi Hong,[a] Wen-Dong Song[b]* and Zao-He Wu[c]

[a]School of Food Science and Technology, Guangdong Ocean University, People's Republic of China, [b]College of Science, Guangdong Ocean University, Zhan Jiang 524088, People's Republic of China, and [c]College of Aquatic Science, Guangdong Ocean University, Zhan Jiang 524088, People's Republic of China
Correspondence e-mail: songwd60@126.com

Received 31 August 2007; accepted 18 December 2007

In the paper by Hong, Song & Wu [*Acta Cryst.* (2007), E**63**, o2296], the scheme shows the wrong structure. The correct scheme is shown below and the compound name is corrected to "poly[[di-μ_2-aqua-diaqua-hemi-μ_6-oxalato-barium(II)] 2,4,6-trinitrophenolate monohydrate", $\{[Ba(C_2O_4)_{0.5}(H_2O)_4]C_6H_2N_3O_7 \cdot H_2O\}_n$.



Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Poly[[tetra-μ_2-aqua-diaqua-μ_6-oxalato-barium(II)] 2,4,6-trinitrophenolate monohydrate]

Peng-Zhi Hong,[a] Wen-Dong Song[b]* and Zao-He Wu[c]

[a]School of Food Science and Technology, Guangdong Ocean University, People's Republic of China, [b]College of Science, Guangdong Ocean University, Zhan Jiang 524088, People's Republic of China, and [c]College of Aquatic Science, Guangdong Ocean University, Zhan Jiang 524088, People's Republic of China
Correspondence e-mail: songwd60@126.com

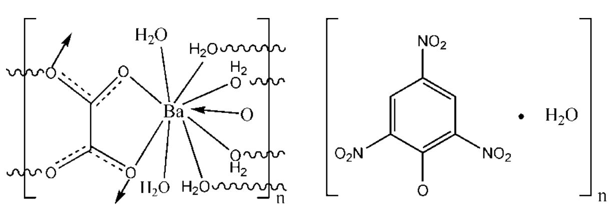
Received 24 April 2007; accepted 3 August 2007

Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.024; *wR* factor = 0.056; data-to-parameter ratio = 14.3.

In the title coordination polymer, $\{[Ba(C_2O_4)(H_2O)_6]\cdot C_6H_2N_3O_7\cdot H_2O\}_n$, each Ba^{II} ion is nine-coordinated by three O atoms from two oxalate ligands, two O atoms from two water molecules and four O atoms from μ_2-bridging aqua ligands, and displays a distorted tricapped trigonal–prismatic geometry. The μ_6-bridging oxalate ligands and μ_2-aqua ligands link Ba^{II} ions to form a neutral layer. The coordinated water molecules link the 2,4,6-trinitrophenolate anions to form a supramolecular network *via* hydrogen-bonding interactions.

Related literature

For related literature, see: Li *et al.* (2003); Pierce-Butler (1982); Ward *et al.* (1984).



Experimental

Crystal data

$[Ba(C_2O_4)(H_2O)_6]C_6H_2N_3O_7\cdot H_2O$
M_r = 499.54
Monoclinic, $P2_1/c$
a = 15.1489 (2) Å
b = 6.5736 (1) Å
c = 15.3111 (2) Å
β = 93.557 (1)°
V = 1521.78 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.70 mm^{-1}
T = 293 (2) K
0.19 × 0.18 × 0.16 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.608, T_{max} = 0.650
13176 measured reflections
3654 independent reflections
3126 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.056
S = 1.03
3654 reflections
256 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WB*···O4	0.834 (17)	2.12 (2)	2.915 (3)	159 (3)
O1*W*—H1*WA*···O5*W*^{i}	0.832 (17)	2.016 (18)	2.837 (3)	169 (3)
O2*W*—H2*WB*···O1^{ii}	0.809 (16)	2.25 (2)	2.961 (3)	146 (3)
O2*W*—H2*WB*···O2^{ii}	0.809 (16)	2.50 (3)	2.974 (3)	118 (2)
O2*W*—H2*WA*···O9^{iii}	0.810 (16)	1.922 (16)	2.697 (3)	160 (3)
O3*W*—H3*WB*···O1^{iv}	0.813 (16)	2.32 (2)	3.051 (3)	149 (3)
O3*W*—H3*WA*···O1*W*	0.808 (16)	1.922 (17)	2.722 (3)	170 (3)
O4*W*—H4*WA*···O5	0.771 (16)	2.250 (17)	3.013 (3)	171 (3)
O4*W*—H4*WB*···O1*W*^{v}	0.796 (16)	2.134 (17)	2.908 (3)	164 (3)
O5*W*—H5*WA*···O1^{vi}	0.812 (16)	1.948 (17)	2.719 (3)	158 (3)
O5*W*—H5*WA*···O7^{vi}	0.812 (16)	2.45 (2)	2.975 (3)	124 (2)
O5*W*—H5*WB*···O4*W*^{vii}	0.812 (16)	2.178 (18)	2.945 (3)	158 (3)

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

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: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

The authors thank the Scientific and Technical Key Leading Project of Guangdong Province of China (grant No. B05119) and Guangdong Ocean University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2010).

References

Brandenburg, K. (2001). *DIAMOND*. Version 3.0. Crystal Impact GbR, Bonn, Germany.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2* (Version 6.12) and *SAINT* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, Y. F., Zhang, T. L., Zhang, J. G., Ma, G. X., Song, J. C., Sun, Y. H. & Yu, K. B. (2003). *Chin. J. Inorg. Chem.* **19**, 861–864.
Pierce-Butler, M. A. (1982). *Acta Cryst.* B**38**, 3097–3100.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Ward, D. L., Popov, A. I. & Poonia, N. S. (1984). *Acta Cryst.* C**40**, 238–241.

supplementary materials

Acta Cryst. (2007). E**63**, m2296 [**doi:10.1107/S1600536807038159**]

Poly[[tetra-μ_2-aqua-diaqua-μ_6-oxalato-barium(II)] 2,4,6-trinitrophenolate monohydrate]

P.-Z. Hong, W.-D. Song and Z.-H. Wu

Comment

2,4,6-trinitrophenolic acid have afforded a large number of O-chelated metal derivates, such as barium (Pierce-Butler, 1982), potassium (Li, *et al.* 2003), sodium (Ward, *et al.*, 1984) and so on.

As illustrated in Fig. 1, in the asymmetric unit of (I) each Ba^{II} centre is nine-coordinated by three carboxyl O atoms from two oxalato ligands, two O atoms from two water molecules and four O atoms from /m$_2$ bridging aqua ligands, and displaying a distorted tricapped trigonal prism geometry. All geometries are general. Via a Ba···Ba interaction between symmetrically related moieties the compound forms polymer structures with a Ba···Ba separation of 6.957 (3) Å that are further extended to a supramolecular network through intermolecular hydrogen bonding interaction among the cationic units, 2,4,6-trinitrophenolate anions and uncoordinated molecules (Table 1 and Fig. 2).

Experimental

The title complex was prepared by the addition of a stoichiometric amount of barium chloride (4.16 g, 20 mmol) and oxalic acid (1.80 g, 20 mmol) to a hot aqueous solution (25 ml) of 2,4,6-trinitrophenolic acid (4.58 g, 30 mmol). The pH was then adjusted to 7.0 to 8.0 with NaOH (1.2 g, 30 mmol). The resulting solution was filtered, and yellow crystals were obtained at room temperature on slow evaporation of the solvent over several days.

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 = 0.82 or 0.85 Å and H···H = 1.29 or 1.39 Å, each within a standard deviation of 0.01 Å. Other H atoms with U_{iso}(H) = 1.5 U_{eq}(O). The highest peak in the difference map is 0.84 (1) Å from Ba1 and the largest hole is 1.13 (2) Å from Ba1.

Figures

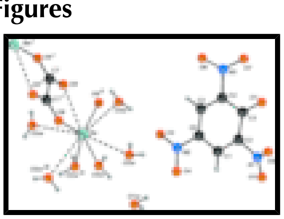


Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms. [Symmetry codes:(i)-x, 1 − y, −z; (ii) −x, −y, −z; (iii) −x, y + 1/2, 1/2 − z; (iv) −x, y − 1/2, 1/2 − z.]

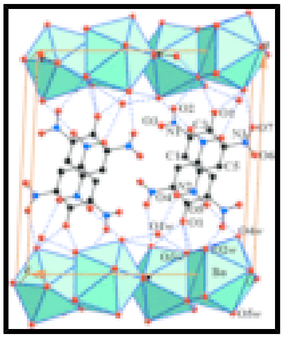


Fig. 2. The unit-cell packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Poly[[di-μ_2-aqua-diaqua-hemi-μ_6-oxalato-barium(II)] 2,4,6-trinitrophenolate monohydrate]

Crystal data

$[Ba(C_2O_4)_{0.5}(H_2O)_4]C_6H_2N_3O_7\cdot H_2O$	F_{000} = 972
M_r = 499.54	D_x = 2.180 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -p_2ybc	Cell parameters from 3600 reflections
a = 15.1489 (2) Å	θ = 1.7–28.0º
b = 6.57360 (10) Å	μ = 2.70 mm^{-1}
c = 15.3111 (2) Å	T = 293 (2) K
β = 93.5570 (10)º	Block, yellow
V = 1521.78 (4) Å^3	0.19 × 0.18 × 0.16 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	3654 independent reflections
Radiation source: fine-focus sealed tube	3126 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 293(2) K	θ_{max} = 28.0º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -20\rightarrow19$
T_{min} = 0.608, T_{max} = 0.650	$k = -8\rightarrow8$
13176 measured reflections	$l = -20\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.024	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.4903P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
3654 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
256 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
14 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	0.009199 (10)	0.090317 (19)	0.144062 (9)	0.02169 (6)
C1	0.53089 (19)	0.0665 (4)	0.32517 (18)	0.0287 (6)
H1	0.5152	0.0558	0.3828	0.034*
C2	0.61794 (18)	0.0706 (4)	0.30611 (17)	0.0272 (6)
C3	0.64955 (18)	0.0795 (4)	0.21936 (17)	0.0264 (6)
C4	0.57696 (19)	0.0866 (4)	0.15341 (17)	0.0286 (6)
C5	0.48959 (19)	0.0906 (4)	0.17056 (18)	0.0291 (6)
H5	0.4462	0.1012	0.1251	0.035*
C6	0.46645 (18)	0.0786 (4)	0.25682 (18)	0.0266 (6)
C7	−0.00848 (17)	0.4258 (3)	−0.03987 (16)	0.0215 (5)
H1WA	0.182 (2)	−0.021 (3)	0.4331 (19)	0.026*
H1WB	0.2387 (13)	0.113 (4)	0.4163 (19)	0.026*
H2WA	0.0900 (16)	−0.317 (4)	0.1881 (15)	0.026*
H2WB	0.1540 (11)	−0.240 (4)	0.2382 (17)	0.026*
H3WA	0.1313 (16)	0.224 (4)	0.3221 (14)	0.026*
H3WB	0.1543 (15)	0.353 (4)	0.2658 (17)	0.026*
H4WA	0.2140 (16)	0.102 (4)	0.1052 (16)	0.026*
H4WB	0.1765 (18)	0.208 (3)	0.0395 (15)	0.026*
H5WA	−0.2039 (15)	0.144 (4)	0.1023 (15)	0.026*
H5WB	−0.1725 (18)	0.123 (4)	0.0273 (12)	0.026*
N1	0.68199 (17)	0.0555 (4)	0.38123 (16)	0.0374 (6)
N2	0.37473 (16)	0.0789 (3)	0.27700 (17)	0.0349 (6)
N3	0.59676 (18)	0.0979 (4)	0.06088 (16)	0.0386 (6)
O1	0.73001 (13)	0.0796 (3)	0.20391 (13)	0.0393 (5)
O2	0.75026 (17)	0.1514 (5)	0.38100 (16)	0.0711 (8)

O3	0.66196 (17)	−0.0536 (4)	0.44163 (15)	0.0607 (7)
O4	0.35790 (16)	0.0651 (4)	0.35365 (16)	0.0553 (7)
O5	0.31768 (15)	0.0929 (4)	0.21685 (17)	0.0556 (7)
O6	0.54645 (17)	0.1997 (4)	0.01244 (15)	0.0593 (7)
O7	0.65884 (16)	0.0004 (5)	0.03584 (15)	0.0611 (7)
O8	−0.00452 (12)	0.2386 (2)	−0.02508 (10)	0.0256 (4)
O9	0.02537 (13)	0.4939 (3)	0.11302 (11)	0.0311 (4)
O1W	0.18547 (15)	0.1042 (4)	0.42656 (16)	0.0439 (5)
O2W	0.10105 (13)	−0.2370 (3)	0.22765 (12)	0.0294 (4)
O3W	0.11131 (13)	0.2932 (3)	0.28179 (13)	0.0322 (4)
O4W	0.17396 (15)	0.1144 (3)	0.07199 (16)	0.0432 (5)
O5W	−0.16202 (14)	0.1761 (4)	0.07469 (14)	0.0397 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba	0.02843 (10)	0.01617 (8)	0.02048 (9)	0.00071 (6)	0.00166 (6)	0.00054 (5)
C1	0.0330 (16)	0.0297 (13)	0.0233 (13)	0.0002 (11)	0.0024 (11)	0.0015 (10)
C2	0.0257 (14)	0.0299 (13)	0.0256 (13)	−0.0018 (11)	−0.0009 (11)	0.0010 (10)
C3	0.0251 (14)	0.0293 (13)	0.0251 (13)	−0.0010 (11)	0.0024 (11)	0.0016 (10)
C4	0.0313 (15)	0.0329 (14)	0.0218 (13)	−0.0024 (11)	0.0033 (11)	0.0007 (10)
C5	0.0278 (15)	0.0323 (14)	0.0266 (13)	−0.0010 (11)	−0.0040 (11)	0.0004 (11)
C6	0.0232 (14)	0.0258 (13)	0.0311 (14)	0.0010 (11)	0.0039 (11)	0.0021 (10)
C7	0.0238 (13)	0.0196 (12)	0.0210 (12)	−0.0016 (10)	0.0005 (10)	0.0006 (9)
N1	0.0300 (14)	0.0570 (16)	0.0251 (12)	0.0012 (12)	0.0001 (10)	0.0040 (11)
N2	0.0250 (13)	0.0368 (13)	0.0430 (15)	0.0013 (10)	0.0034 (11)	0.0021 (10)
N3	0.0366 (15)	0.0548 (16)	0.0241 (12)	−0.0148 (13)	0.0011 (11)	−0.0023 (11)
O1	0.0242 (11)	0.0616 (14)	0.0322 (11)	−0.0026 (10)	0.0033 (9)	0.0011 (9)
O2	0.0423 (15)	0.128 (2)	0.0418 (14)	−0.0344 (16)	−0.0089 (12)	0.0092 (15)
O3	0.0463 (15)	0.097 (2)	0.0383 (13)	−0.0038 (13)	−0.0067 (11)	0.0281 (13)
O4	0.0367 (14)	0.0888 (19)	0.0424 (14)	0.0053 (12)	0.0174 (11)	0.0069 (12)
O5	0.0272 (12)	0.0817 (19)	0.0568 (15)	0.0000 (11)	−0.0067 (11)	0.0038 (12)
O6	0.0700 (18)	0.0735 (17)	0.0332 (12)	−0.0032 (14)	−0.0053 (12)	0.0162 (12)
O7	0.0420 (15)	0.107 (2)	0.0355 (13)	0.0007 (15)	0.0117 (11)	−0.0187 (14)
O8	0.0371 (11)	0.0156 (8)	0.0241 (9)	−0.0007 (8)	0.0018 (8)	−0.0003 (6)
O9	0.0480 (13)	0.0202 (9)	0.0241 (9)	−0.0037 (8)	−0.0060 (8)	0.0018 (7)
O1W	0.0266 (12)	0.0562 (14)	0.0490 (13)	0.0089 (11)	0.0037 (10)	0.0072 (11)
O2W	0.0300 (11)	0.0311 (10)	0.0269 (10)	0.0046 (9)	−0.0011 (8)	−0.0014 (8)
O3W	0.0325 (12)	0.0333 (11)	0.0304 (10)	−0.0008 (9)	−0.0016 (9)	0.0039 (8)
O4W	0.0305 (12)	0.0545 (14)	0.0440 (14)	0.0009 (10)	−0.0018 (10)	0.0108 (10)
O5W	0.0306 (12)	0.0619 (14)	0.0270 (11)	−0.0074 (11)	0.0042 (9)	−0.0005 (10)

Geometric parameters (Å, °)

Ba—O9	2.709 (2)	C5—C6	1.390 (4)
Ba—O8	2.763 (2)	C5—H5	0.9300
Ba—O4W	2.795 (2)	C6—N2	1.442 (4)
Ba—O5W	2.799 (2)	C7—O9^{v}	1.250 (3)

Ba—O2W	2.825 (2)	C7—O8	1.252 (3)
Ba—O8^{i}	2.826 (2)	C7—C7^{v}	1.571 (5)
Ba—O3W	2.866 (2)	N1—O2	1.212 (3)
Ba—O2W^{ii}	2.888 (2)	N1—O3	1.223 (3)
Ba—O3W^{iii}	2.949 (2)	N2—O4	1.220 (3)
Ba—Ba^{iv}	6.957 (3)	N2—O5	1.227 (3)
Ba—Ba^{i}	4.5603 (3)	N3—O7	1.219 (3)
Ba—Ba^{ii}	4.6386 (2)	N3—O6	1.228 (3)
Ba—Ba^{iii}	4.6386 (2)	O1W—H1WA	0.832 (17)
C1—C2	1.368 (4)	O1W—H1WB	0.834 (17)
C1—C6	1.388 (4)	O2W—H2WA	0.810 (16)
C1—H1	0.9300	O2W—H2WB	0.809 (16)
C2—C3	1.441 (4)	O3W—H3WA	0.808 (16)
C2—N1	1.461 (3)	O3W—H3WB	0.813 (16)
C3—O1	1.256 (3)	O4W—H4WA	0.771 (16)
C3—C4	1.447 (4)	O4W—H4WB	0.796 (16)
C4—C5	1.366 (4)	O5W—H5WA	0.812 (16)
C4—N3	1.468 (4)	O5W—H5WB	0.812 (16)

O9—Ba—O8	59.49 (5)	O3W—Ba—O3W^{iii}	110.10 (3)
O9—Ba—O4W	77.44 (6)	O2W^{ii}—Ba—O3W^{iii}	66.46 (5)
O8—Ba—O4W	68.10 (6)	C2—C1—C6	118.7 (3)
O9—Ba—O5W	80.09 (6)	C1—C2—C3	125.3 (2)
O8—Ba—O5W	63.84 (6)	C1—C2—N1	115.6 (2)
O4W—Ba—O5W	131.91 (6)	C3—C2—N1	119.1 (2)
O9—Ba—O2W	141.07 (6)	O1—C3—C2	123.7 (2)
O8—Ba—O2W	134.40 (5)	O1—C3—C4	125.0 (3)
O4W—Ba—O2W	78.19 (6)	C2—C3—C4	111.3 (2)
O5W—Ba—O2W	138.08 (6)	C5—C4—C3	124.8 (3)
O9—Ba—O8^{i}	129.44 (5)	C5—C4—N3	116.3 (2)
O8—Ba—O8^{i}	70.63 (5)	C3—C4—N3	118.9 (3)
O4W—Ba—O8^{i}	77.07 (6)	C4—C5—C6	119.1 (2)
O5W—Ba—O8^{i}	85.63 (6)	C1—C6—C5	120.8 (3)
O2W—Ba—O8^{i}	72.61 (5)	C1—C6—N2	118.7 (3)
O9—Ba—O3W	67.85 (5)	C5—C6—N2	120.5 (2)
O8—Ba—O3W	122.09 (5)	O9^{v}—C7—O8	125.6 (2)
O4W—Ba—O3W	79.03 (6)	O9^{v}—C7—C7^{v}	116.6 (2)
O5W—Ba—O3W	129.11 (6)	O8—C7—C7^{v}	117.8 (2)
O2W—Ba—O3W	78.05 (5)	O2—N1—O3	124.0 (3)
O8^{i}—Ba—O3W	145.21 (5)	O2—N1—C2	119.2 (2)
O9—Ba—O2W^{ii}	78.28 (6)	O3—N1—C2	116.8 (2)
O8—Ba—O2W^{ii}	119.06 (5)	O4—N2—O5	123.2 (3)
O4W—Ba—O2W^{ii}	144.51 (6)	O4—N2—C6	117.9 (2)
O5W—Ba—O2W^{ii}	67.51 (6)	O5—N2—C6	118.9 (3)
O2W—Ba—O2W^{ii}	106.29 (4)	O7—N3—O6	123.9 (3)

O8^{i}—Ba—O2W^{ii}	138.31 (5)	O7—N3—C4	119.0 (3)
O3W—Ba—O2W^{ii}	67.99 (5)	O6—N3—C4	117.0 (3)
O9—Ba—O3W^{iii}	141.37 (6)	H1WA—O1W—H1WB	99 (3)
O8—Ba—O3W^{iii}	125.61 (5)	H2WA—O2W—H2WB	107 (2)
O4W—Ba—O3W^{iii}	141.16 (6)	H3WA—O3W—H3WB	104 (2)
O5W—Ba—O3W^{iii}	72.43 (6)	H4WA—O4W—H4WB	116 (2)
O2W—Ba—O3W^{iii}	67.69 (6)	H5WA—O5W—H5WB	104 (2)
O8^{i}—Ba—O3W^{iii}	75.52 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WB···O4	0.834 (17)	2.12 (2)	2.915 (3)	159 (3)
O1W—H1WA···O5W^{iii}	0.832 (17)	2.016 (18)	2.837 (3)	169 (3)
O2W—H2WB···O1^{vi}	0.809 (16)	2.25 (2)	2.961 (3)	146 (3)
O2W—H2WB···O2^{vi}	0.809 (16)	2.50 (3)	2.974 (3)	118 (2)
O2W—H2WA···O9^{vii}	0.810 (16)	1.922 (16)	2.697 (3)	160 (3)
O3W—H3WB···O1^{viii}	0.813 (16)	2.32 (2)	3.051 (3)	149 (3)
O3W—H3WA···O1W	0.808 (16)	1.922 (17)	2.722 (3)	170 (3)
O4W—H4WA···O5	0.771 (16)	2.250 (17)	3.013 (3)	171 (3)
O4W—H4WB···O1W^{ix}	0.796 (16)	2.134 (17)	2.908 (3)	164 (3)
O5W—H5WA···O1^{x}	0.812 (16)	1.948 (17)	2.719 (3)	158 (3)
O5W—H5WA···O7^{x}	0.812 (16)	2.45 (2)	2.975 (3)	124 (2)
O5W—H5WB···O4W^{i}	0.812 (16)	2.178 (18)	2.945 (3)	158 (3)

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

Fig. 1

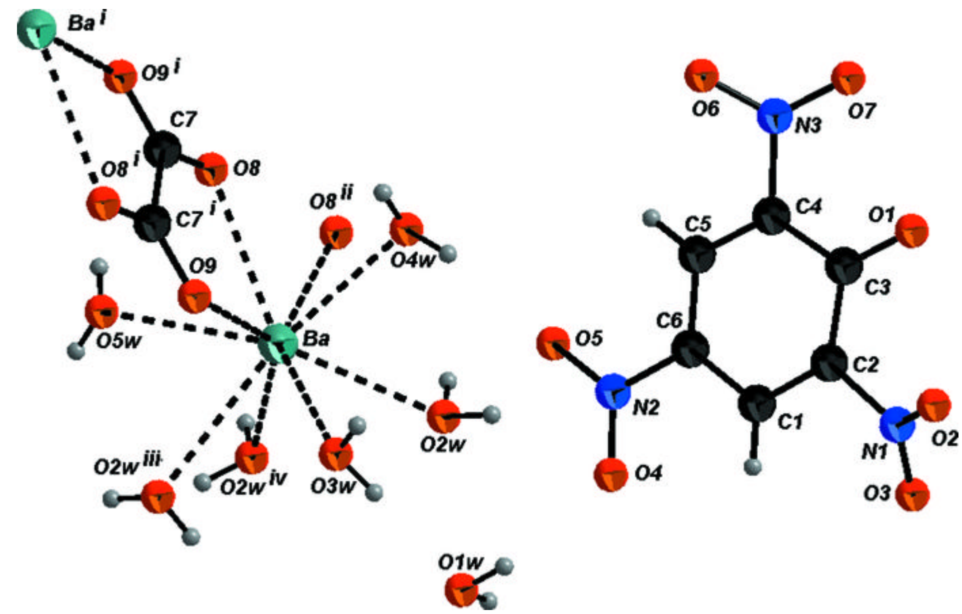

Ba i
O9 i
C7
O8 i
O8
C7 i
O8 ii
O4w
O9
O5w
Ba
O2w
O2w iii
O2w iv
O3w
O1w
O6
O7
N3
C4
C5
O1
C3
C6
O5
C2
N2
C1
N1
O2
O4
O3

Fig. 2