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catena-Poly[[[triaquabarium(II)]-di-μ-2,4,6-trinitrophenolato-κ^3O:O',O'';-κ^3O,O':O''] benzimidazole disolvate]

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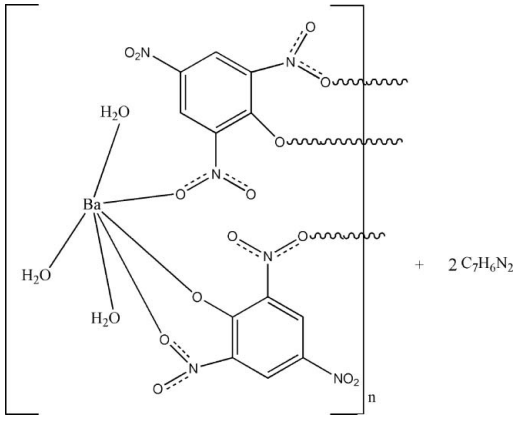
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.049; data-to-parameter ratio = 12.5.

In the title complex, $\{[Ba(C_6H_2N_3O_7)_2(H_2O)_3]\cdot 2C_7H_6N_2\}_n$, the Ba^{II} coordination polyhedron is defined by six O atoms from four 2,4,6-trinitrophenolate ligands and three water molecules, displaying a distorted monocapped square-antiprismatic geometry. Both the Ba atom and one of the coordinated water molecules lie on a twofold axis. The compound forms an infinite chain parallel to the c axis through κ^3-bridging 2,4,6-trinitrophenolate ligands to the metal atoms. A supramolecular network is formed *via* hydrogen bonding and π–π interactions involving both the chains and benzimidazole solvent molecules. The face-to-face and centroid– centroid distances between parallel 2,4,6-trinitrophenolate and benzimidazole rings of neighboring complexes are 3.509 (3) and 3.613 (2) Å, respectively.

Related literature

For related literature, see: Choi & Jeon (2003); Gu *et al.* (2004); Tao *et al.* (2000).



Experimental

Crystal data

$[Ba(C_6H_2N_3O_7)_2(H_2O)_3]\cdot 2C_7H_6N_2$
M_r = 882.87
Monoclinic, $C2/c$
a = 30.4215 (6) Å
b = 6.7394 (1) Å
c = 16.6695 (3) Å
β = 107.950 (1)°
V = 3251.27 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.797
11230 measured reflections
3176 independent reflections
2965 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.049
S = 1.03
3176 reflections
254 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ba1—O5	2.6451 (14)	Ba1—O2W	2.8484 (16)
Ba1—O1W	2.683 (2)	Ba1—O3	2.9596 (17)
Ba1—O7^{i}	2.8184 (15)		

Symmetry code: (i) $x, -y+1, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O2W^{ii}	0.80 (2)	2.02 (2)	2.816 (2)	171 (6)
O2W—H2W···N1^{iii}	0.83 (2)	1.98 (2)	2.812 (2)	174 (2)
O2W—H3W···O5	0.80 (2)	2.16 (2)	2.768 (2)	133 (2)
O2W—H3W···O6	0.80 (2)	2.34 (2)	3.058 (2)	148 (2)
N2—H2A···O8^{iv}	0.86	2.13	2.987 (2)	174

Symmetry codes: (ii) $-x, y-1, -z+\frac{1}{2}$; (iii) $-x, y, -z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

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, 2004); 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: BG2054).

  doi:10.1107/S1600536807024610

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supplementary materials

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catena-Poly[[[triaquabarium(II)]-di-μ-2,4,6-trinitrophenolato-$\kappa^3O:O',O'';\kappa^3O,O':O''$] benzimidazole disolvate]

D.-Y. Ma and G.-H. Deng

Comment

Molecular self-assembly of supramolecular architectures has received much attention during recent decades (Tao *et al.*, 2000; Choi & Jeon, 2003). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metal ions and the bridging building blocks, as well as on the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions. In this sense, 2,4,6-trinitrophenolate is an excellent candidante for the construction of supramolecular complexes, since it not only displays multiple coordination modes but also can form regular hydrogen bonds by functioning both as hydrogen-bond donor and acceptor (Gu *et al.*, 2004). In the present paper, we report the novel title Ba polymer (I).

Fig. 1 shows its molecular diagram: the Ba^{II} atom lies on a two fold axis and presents a distorted mono-capped square antiprism geometry, defined by six O atoms from four 2,4,6-trinitrophenolate ligands, and three water molecules, one of which is also bisected by the diad. The compound forms an infinite chain parallel to the *c* axis through κ_3 bridging 2,4,6-trinitrophenolate ligands to the metal atoms, with the adjacent Ba···Ba distance being 8.362 (3) /%A. Inter/intramolecular (O—H···O and N—H···O) hydrogen bonding (Table 2) and π···π interactions involving both the chains and independent benzimidazole molecules stabilize the supramolecular network (Fig. 2). The face-to-face and centroid-centroid distances between parallel 2,4,6-trinitrophenolate and benzimidazole of neighboring complexes are 3.509 (3) and 3.613 (2) Å, respectively.

Experimental

The title complex was prepared by the addition of a stoichiometric amount of barium chloride (20 mmol) and benzimidazole (20 mmol) to a hot aqueous solution(25 ml) of 2,4,6-trinitrophenolate (20 mmol). the PH was then adjusted to 7.0 to 8.0 with NaOH (30 mmol)·The resulting solution was filtered, and yellow single crystals were obtained at room temperature over several days. (yield, 58%).

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. Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 (1) Å and H···H = 1.29 (1) Å. In all cases, U_{iso}(H) = 1.2 U_{eq}(Host).

Figures

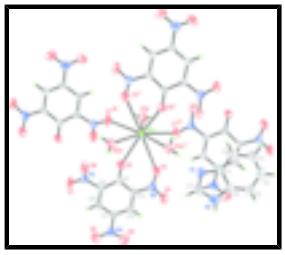

Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 30% probability displacement ellipsoids. Symmetry code: (i) −*x*, *y*, 1/2 − *z*; (ii) *x*, 1 − *y*, −1/2 + *z*; (iii) −*x*, 1 − *y*, 1 − *z*.

Fig. 2. A packing view of (I), Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Ba(C_6H_2N_3O_7)_2(H_2O)_3].2C_7H_6N_2$	F_{000} = 1756
M_r = 882.87	D_x = 1.804 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3200 reflections
a = 30.4215 (6) Å	θ = 1.7–28.0º
b = 6.73940 (10) Å	μ = 1.32 mm^{-1}
c = 16.6695 (3) Å	*T* = 293 (2) K
β = 107.9500 (10)º	Block, yellow
V = 3251.27 (10) Å^3	0.20 × 0.18 × 0.18 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	3176 independent reflections
Radiation source: fine-focus sealed tube	2965 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −37→37
T_{min} = 0.779, T_{max} = 0.797	*k* = −8→8
11230 measured reflections	*l* = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.020$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 2.8124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3176 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
254 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
4 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}	Occ. (<1)
Ba1	0.0000	0.54969 (3)	0.2500	0.02678 (6)	
C1	0.12475 (6)	0.8786 (3)	0.04517 (13)	0.0305 (4)	
C2	0.09690 (7)	0.8776 (3)	−0.03851 (14)	0.0385 (5)	
H2	0.0649	0.8729	−0.0523	0.046*	
C3	0.11831 (9)	0.8839 (4)	−0.10030 (15)	0.0479 (6)	
H3	0.1003	0.8835	−0.1566	0.058*	
C4	0.16600 (10)	0.8909 (4)	−0.08066 (17)	0.0533 (6)	
H4	0.1791	0.8943	−0.1242	0.064*	
C5	0.19433 (8)	0.8930 (4)	0.00113 (18)	0.0493 (6)	
H5	0.2263	0.8986	0.0140	0.059*	
C6	0.17305 (7)	0.8863 (3)	0.06404 (14)	0.0359 (5)	
C7	0.15304 (9)	0.8749 (4)	0.17941 (15)	0.0477 (6)	
H7	0.1558	0.8714	0.2365	0.057*	
C8	0.08615 (6)	0.6307 (3)	0.46576 (12)	0.0271 (4)	
C9	0.08875 (6)	0.6439 (3)	0.55372 (12)	0.0272 (4)	
C10	0.12886 (6)	0.6317 (3)	0.61992 (12)	0.0292 (4)	
H10	0.1282	0.6347	0.6753	0.035*	
C11	0.17024 (6)	0.6148 (3)	0.60218 (12)	0.0315 (4)	
C12	0.17172 (6)	0.6059 (3)	0.52008 (13)	0.0313 (4)	
H12	0.1999	0.5963	0.5096	0.038*	
C13	0.13161 (6)	0.6113 (3)	0.45470 (12)	0.0279 (4)	
N1	0.11318 (6)	0.8717 (3)	0.11972 (11)	0.0399 (4)	

N2	0.18963 (6)	0.8836 (3)	0.15040 (12)	0.0473 (5)	
H2A	0.2182	0.8869	0.1805	0.057*	
N3	0.04662 (5)	0.6730 (3)	0.57559 (10)	0.0339 (4)	
N4	0.21295 (6)	0.6097 (3)	0.67093 (12)	0.0424 (5)	
N5	0.13605 (6)	0.6021 (3)	0.37039 (11)	0.0360 (4)	
O3	0.10196 (6)	0.5831 (3)	0.30871 (10)	0.0606 (5)	
O4	0.17466 (6)	0.6120 (3)	0.36322 (11)	0.0598 (5)	
O5	0.04921 (5)	0.6328 (3)	0.40711 (9)	0.0435 (4)	
O6	0.01290 (5)	0.7470 (3)	0.52530 (10)	0.0633 (6)	
O7	0.04724 (6)	0.6278 (3)	0.64730 (10)	0.0519 (4)	
O8	0.21155 (6)	0.6352 (3)	0.74293 (10)	0.0619 (5)	
O9	0.24904 (5)	0.5800 (4)	0.65494 (12)	0.0718 (6)	
O1W	0.0000	0.1516 (4)	0.2500	0.0525 (6)	
H1W	0.010 (2)	0.076 (7)	0.224 (3)	0.063*	0.50
O2W	−0.03027 (5)	0.8540 (3)	0.33929 (9)	0.0395 (3)	
H2W	−0.0537 (6)	0.862 (4)	0.3550 (14)	0.047*	
H3W	−0.0098 (6)	0.828 (4)	0.3817 (12)	0.047*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.02865 (9)	0.03324 (10)	0.01903 (9)	0.000	0.00817 (6)	0.000
C1	0.0307 (9)	0.0268 (10)	0.0341 (11)	−0.0013 (8)	0.0100 (8)	0.0007 (9)
C2	0.0359 (10)	0.0342 (11)	0.0396 (12)	−0.0017 (9)	0.0032 (9)	0.0005 (10)
C3	0.0684 (16)	0.0406 (13)	0.0320 (12)	0.0008 (12)	0.0115 (11)	0.0007 (10)
C4	0.0746 (17)	0.0451 (14)	0.0534 (16)	0.0002 (13)	0.0391 (14)	0.0019 (12)
C5	0.0383 (12)	0.0454 (14)	0.0713 (18)	−0.0008 (10)	0.0275 (12)	0.0008 (13)
C6	0.0314 (10)	0.0311 (11)	0.0421 (12)	0.0003 (8)	0.0068 (9)	0.0010 (9)
C7	0.0648 (15)	0.0461 (14)	0.0298 (12)	−0.0031 (12)	0.0113 (11)	0.0018 (11)
C8	0.0278 (9)	0.0288 (10)	0.0240 (9)	−0.0007 (8)	0.0071 (7)	−0.0014 (8)
C9	0.0287 (9)	0.0290 (10)	0.0253 (9)	−0.0015 (8)	0.0103 (7)	0.0002 (8)
C10	0.0345 (10)	0.0312 (10)	0.0212 (9)	−0.0022 (8)	0.0077 (8)	0.0011 (8)
C11	0.0279 (9)	0.0356 (11)	0.0262 (10)	−0.0016 (8)	0.0013 (8)	0.0015 (9)
C12	0.0277 (9)	0.0356 (11)	0.0319 (11)	0.0001 (8)	0.0111 (8)	−0.0001 (9)
C13	0.0319 (9)	0.0304 (10)	0.0221 (9)	0.0000 (8)	0.0095 (8)	0.0002 (8)
N1	0.0440 (10)	0.0407 (10)	0.0374 (10)	−0.0024 (9)	0.0162 (8)	0.0013 (9)
N2	0.0378 (10)	0.0503 (12)	0.0425 (11)	−0.0018 (9)	−0.0044 (8)	0.0017 (10)
N3	0.0321 (8)	0.0442 (11)	0.0277 (9)	−0.0011 (8)	0.0125 (7)	−0.0029 (8)
N4	0.0318 (9)	0.0544 (12)	0.0343 (10)	−0.0038 (8)	0.0001 (8)	0.0048 (9)
N5	0.0399 (9)	0.0436 (11)	0.0277 (9)	0.0011 (8)	0.0150 (8)	0.0003 (8)
O3	0.0454 (9)	0.1133 (18)	0.0223 (8)	−0.0046 (10)	0.0093 (7)	−0.0052 (9)
O4	0.0453 (9)	0.1017 (16)	0.0418 (9)	−0.0006 (10)	0.0271 (8)	−0.0007 (10)
O5	0.0289 (7)	0.0726 (11)	0.0250 (7)	0.0029 (7)	0.0024 (6)	−0.0088 (8)
O6	0.0397 (8)	0.1134 (17)	0.0381 (9)	0.0293 (10)	0.0138 (7)	0.0088 (10)
O7	0.0503 (9)	0.0778 (12)	0.0364 (9)	0.0007 (9)	0.0266 (7)	0.0122 (9)
O8	0.0438 (9)	0.1064 (16)	0.0276 (9)	−0.0049 (10)	−0.0006 (7)	0.0031 (10)
O9	0.0275 (8)	0.130 (2)	0.0517 (11)	0.0076 (10)	0.0033 (8)	−0.0012 (11)
O1W	0.0769 (17)	0.0340 (13)	0.0618 (17)	0.000	0.0435 (14)	0.000

O2W	0.0390 (8)	0.0474 (9)	0.0345 (8)	0.0063 (7)	0.0152 (6)	0.0028 (8)

Geometric parameters (Å, °)

Ba1—O5	2.6451 (14)	C8—O5	1.242 (2)
Ba1—O5^{i}	2.6451 (14)	C8—C9	1.447 (3)
Ba1—O1W	2.683 (2)	C8—C13	1.456 (3)
Ba1—O7^{ii}	2.8184 (15)	C9—C10	1.372 (3)
Ba1—O7^{iii}	2.8184 (15)	C9—N3	1.450 (2)
Ba1—O2W^{i}	2.8484 (16)	C10—C11	1.384 (3)
Ba1—O2W	2.8484 (16)	C10—H10	0.9300
Ba1—O3	2.9596 (17)	C11—C12	1.384 (3)
Ba1—O3^{i}	2.9596 (17)	C11—N4	1.444 (2)
C1—C2	1.391 (3)	C12—C13	1.363 (3)
C1—N1	1.393 (3)	C12—H12	0.9300
C1—C6	1.406 (3)	C13—N5	1.454 (2)
C2—C3	1.379 (3)	N2—H2A	0.8600
C2—H2	0.9300	N3—O6	1.214 (2)
C3—C4	1.386 (4)	N3—O7	1.228 (2)
C3—H3	0.9300	N4—O9	1.223 (2)
C4—C5	1.370 (4)	N4—O8	1.226 (2)
C4—H4	0.9300	N5—O4	1.219 (2)
C5—C6	1.393 (3)	N5—O3	1.221 (2)
C5—H5	0.9300	O7—Ba1^{iii}	2.8184 (15)
C6—N2	1.371 (3)	O1W—H1W	0.80 (2)
C7—N1	1.310 (3)	O2W—H2W	0.83 (2)
C7—N2	1.345 (3)	O2W—H3W	0.80 (2)
C7—H7	0.9300		
O5—Ba1—O5^{i}	155.56 (8)	C2—C3—H3	119.1
O5—Ba1—O1W	102.22 (4)	C4—C3—H3	119.1
O5^{i}—Ba1—O1W	102.22 (4)	C5—C4—C3	121.8 (2)
O5—Ba1—O7^{ii}	116.89 (5)	C5—C4—H4	119.1
O5^{i}—Ba1—O7^{ii}	74.18 (5)	C3—C4—H4	119.1
O1W—Ba1—O7^{ii}	64.88 (4)	C4—C5—C6	116.9 (2)
O5—Ba1—O7^{iii}	74.18 (5)	C4—C5—H5	121.5
O5^{i}—Ba1—O7^{iii}	116.89 (5)	C6—C5—H5	121.5
O1W—Ba1—O7^{iii}	64.88 (4)	N2—C6—C5	133.3 (2)
O7^{ii}—Ba1—O7^{iii}	129.77 (8)	N2—C6—C1	104.79 (19)
O5—Ba1—O2W^{i}	100.92 (5)	C5—C6—C1	122.0 (2)
O5^{i}—Ba1—O2W^{i}	60.38 (5)	N1—C7—N2	113.7 (2)
O1W—Ba1—O2W^{i}	136.05 (3)	N1—C7—H7	123.1
O7^{ii}—Ba1—O2W^{i}	71.38 (5)	N2—C7—H7	123.1
O7^{iii}—Ba1—O2W^{i}	158.50 (5)	O5—C8—C9	123.43 (17)
O5—Ba1—O2W	60.38 (5)	O5—C8—C13	124.44 (17)
O5^{i}—Ba1—O2W	100.92 (5)	C9—C8—C13	112.11 (16)

O1W—Ba1—O2W	136.05 (3)	C10—C9—C8	124.65 (17)
O7^{ii}—Ba1—O2W	158.50 (5)	C10—C9—N3	116.22 (16)
O7^{iii}—Ba1—O2W	71.38 (5)	C8—C9—N3	119.13 (16)
O2W^{i}—Ba1—O2W	87.90 (6)	C9—C10—C11	118.37 (17)
O5—Ba1—O3	56.00 (4)	C9—C10—H10	120.8
O5^{i}—Ba1—O3	121.80 (4)	C11—C10—H10	120.8
O1W—Ba1—O3	94.37 (4)	C10—C11—C12	121.58 (17)
O7^{ii}—Ba1—O3	63.55 (5)	C10—C11—N4	119.20 (18)
O7^{iii}—Ba1—O3	120.67 (5)	C12—C11—N4	119.21 (18)
O2W^{i}—Ba1—O3	69.10 (5)	C13—C12—C11	119.69 (17)
O2W—Ba1—O3	104.30 (5)	C13—C12—H12	120.2
O5—Ba1—O3^{i}	121.80 (4)	C11—C12—H12	120.2
O5^{i}—Ba1—O3^{i}	56.00 (4)	C12—C13—N5	116.40 (16)
O1W—Ba1—O3^{i}	94.37 (4)	C12—C13—C8	123.52 (17)
O7^{ii}—Ba1—O3^{i}	120.67 (5)	N5—C13—C8	120.06 (16)
O7^{iii}—Ba1—O3^{i}	63.55 (5)	C7—N1—C1	104.35 (18)
O2W^{i}—Ba1—O3^{i}	104.30 (5)	C7—N2—C6	107.51 (18)
O2W—Ba1—O3^{i}	69.10 (5)	C7—N2—H2A	126.2
O3—Ba1—O3^{i}	171.26 (9)	C6—N2—H2A	126.2
O5—Ba1—H3W	44.8 (3)	O6—N3—O7	122.01 (17)
O5^{i}—Ba1—H3W	116.3 (3)	O6—N3—C9	120.42 (16)
O1W—Ba1—H3W	129.2 (5)	O7—N3—C9	117.50 (16)
O7^{ii}—Ba1—H3W	154.5 (4)	O9—N4—O8	122.71 (18)
O7^{iii}—Ba1—H3W	68.5 (5)	O9—N4—C11	118.65 (19)
O2W^{i}—Ba1—H3W	93.0 (5)	O8—N4—C11	118.64 (18)
O2W—Ba1—H3W	15.7 (3)	O4—N5—O3	121.14 (18)
O3—Ba1—H3W	92.3 (3)	O4—N5—C13	118.16 (17)
O3^{i}—Ba1—H3W	82.1 (3)	O3—N5—C13	120.70 (16)
C2—C1—N1	130.62 (18)	N5—O3—Ba1	144.86 (13)
C2—C1—C6	119.76 (19)	C8—O5—Ba1	151.16 (13)
N1—C1—C6	109.62 (18)	N3—O7—Ba1^{iii}	147.01 (14)
C3—C2—C1	117.8 (2)	Ba1—O1W—H1W	130 (4)
C3—C2—H2	121.1	Ba1—O2W—H2W	131.0 (19)
C1—C2—H2	121.1	Ba1—O2W—H3W	90.9 (18)
C2—C3—C4	121.7 (2)	H2W—O2W—H3W	104.2 (19)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O2W^{iv}	0.80 (2)	2.02 (2)	2.816 (2)	171 (6)
O2W—H2W···N1^{i}	0.83 (2)	1.98 (2)	2.812 (2)	174 (2)
O2W—H3W···O5	0.80 (2)	2.16 (2)	2.768 (2)	133 (2)
O2W—H3W···O6	0.80 (2)	2.34 (2)	3.058 (2)	148 (2)

N2—H2A···O8^{v}	0.86	2.13	2.987 (2)	174

Symmetry codes: (iv) −*x*, *y*−1, −*z*+1/2; (i) −*x*, *y*, −*z*+1/2; (v) −*x*+1/2, −*y*+3/2, −*z*+1.

Fig. 1

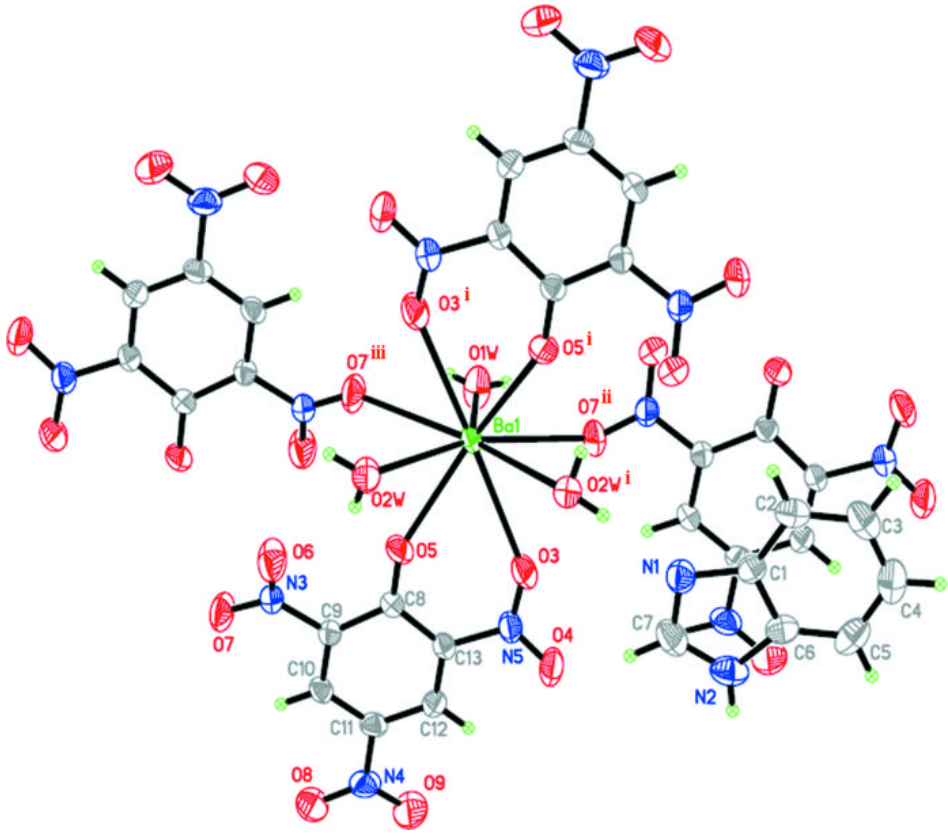

Fig. 2