Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua[7,11:19,23-dinitrilo-1,5,13,17-tetraazacyclotetracosa-1(24),5,7,9,-12,17,20,22-octaene]bis(perchlorato-κ^2O,O')barium(II) monohydrate

Rebecca Dennett, Leanne James and Vickie McKee*

Chemistry Department, Loughborough University, Loughborough, Leicestershire LE11 3TU, England
Correspondence e-mail: v.mckee@lboro.ac.uk

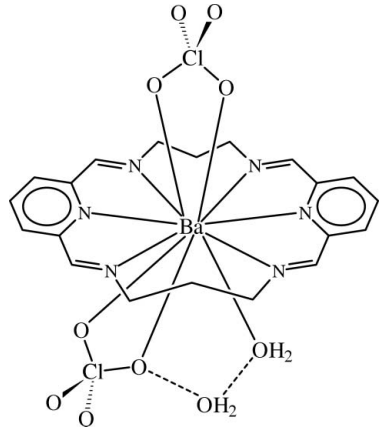
Received 15 May 2007; accepted 16 May 2007

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; H-atom completeness 85%; disorder in main residue; R factor = 0.023; wR factor = 0.057; data-to-parameter ratio = 20.3.

The title complex, $[Ba(ClO_4)_2(C_{20}H_{22}N_6)(H_2O)]\cdot H_2O$, contains an 11-coordinate barium ion, coordinated by a folded hexadentate macrocycle, two bidentate perchlorate anions and a water molecule. The coordinated water molecule and one of the perchlorate anions are disordered about a twofold axis running through the complex. Hydrogen-bonded sheets are linked in the third dimension by π–π stacking (the mean interplanar distance is 3.441 Å).

Related literature

In 1990, the structure of a complex formulated as $[Ba(C_{20}H_{22}N_6)(ClO_4)_2(C_2H_5OH)]$, (II), was determined at ambient temperature and refined in space group *Aa* to a value of $R = 0.080$ for data with $I > 2\sigma(I)$ (Harding *et al.*, 1990). Low-temperature data for the title complex gave a unit cell apparently isomorphous with that of (II) and a similar solution in *Cc*, but the refinement was poor (see Supplementary Material). Solution in *C2/c*, however, gave a much better refinement for a model with disorder between one coordinated perchlorate anion and a coordinated water molecule across the twofold axis. While it is possible that both the title complex and (II) could differ in the coordinated solvent present and still have very similar unit cells, it is also possible that the complexes are the same and that the earlier structure should be re-interpreted.



Experimental

Crystal data

$[Ba)(ClO_4)_2(C_{20}H_{22}N_6(H_2O)]\cdot H_2O$
M_r = 718.71
Monoclinic, $C2/c$
a = 14.5247 (8) Å
b = 12.0634 (6) Å
c = 15.8698 (8) Å
β = 104.157 (1)°
V = 2696.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.74 mm^{-1}
T = 150 (2) K
0.51 × 0.31 × 0.13 mm

Data collection

Bruker APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.472, T_{max} = 0.806
16000 measured reflections
4334 independent reflections
4120 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.057
S = 1.19
4334 reflections
213 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

The H atoms of these water molecules were not located.

$D\cdots A$	$D\cdots A$	$D\cdots A$	$D\cdots A$
O1$W\cdots$O2W	2.761 (6)	O2$W\cdots$O6	2.904 (7)
O1$W\cdots$O8^{i}	2.866 (5)	O2$W\cdots$O2^{ii}	2.846 (5)

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

Data collection: *APEX2* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2395).

  doi:10.1107/S1600536807024270

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Harding, C., McDowell, D., Nelson, J., Raghunathan, S., Stevenson, C., Drew, M. G. B. & Yates, P. C. (1990). *J. Chem. Soc. Dalton Trans.* pp. 2521–2533.
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supplementary materials

Acta Cryst. (2007). E**63**, m1720-m1721 [**doi:10.1107/S1600536807024270**]

Aqua[7,11:19,23-dinitrilo-1,5,13,17-tetraazacyclotetracosa-1(24),5,7,9,12,17,20,22-octaene]bis(perchlorato-κ^2O,O')barium(II) monohydrate

R. Dennett, L. James and V. McKee

Comment

The stucture of the title compound, $[Ba(C_{20}H_{22}N_6)(ClO_4)_2(H_2O)]\cdot H_2O$, (I), was solved in *C2/c* and is shown in Fig. 1. The barium ion is 11-coordinate; it is bonded to all six N donors of the macrocycle, which is folded to accommodate the metal (N1—Ba—$N1^i$, 130.69 (6)°). Two bidentate perchlorate anions are also coordinated, one on each side of the macrocycle, and the coordination sphere is completed by a water molecule (O1W) on the convex side. A non-coordinated water molecule (O2W) is H-bonded to O1W and to the perchlorate ion. A 2-fold axis runs through Ba1 and Cl1 and this requires that the perchlorate/water assembly on the convex face of the macrocycle is disordered with equal occupancy of two positions related by the 2-fold axis, as shown in Fig. 2. There is also a minor disorder in the saturated portion of the macrocycle at C9; this was modelled as 9:1 occupancy of two related sites.

The water molecules link the complex molecules into two-dimensional sheets perpendicular to *a* through further H-bonding (Table 1). The disorder of the groups coordinated on the convex face of the macrocycle gives rise to two possible H-bonding nets related by a 2-fold axis, one of these is shown in Fig. 3. The principal interaction between adjacent layers is π-π stacking of the pyridine-imine unit with the same section of an adjacent molecule under symmetry operation (iv) $-x - 1/2, -y + 3/2, -z + 1$ (Fig. 4). The mean interplanar distance between the overlapping sections (N1, N2, C1 – C6) is 3.441 Å. Interactions between layers are not affected significantly by the disorder within the two-dimensional H-bonded sheets, so the structure can be viewed as a random stack of the two H-bonded layers.

The structure was initially solved in *Cc* as the statistics indicated a non-centrosymmetric space group (possibly an artefact due to the presence of the heavy Ba atom). There was disorder evident on the convex side of the macrocycle, racemic twinning was indicated, the Flack parameter refined to 0.43 (2), and the anisotropic refinement required a series of restraints to prevent atoms going non-positive definite. Hence, the centrosymmetric solution was preferred.

Experimental

Complex (I), $[Ba(C_{20}H_{22}N_6)(ClO_4)_2(H_2O)]H_2O$, was prepared as reported previously (Harding *et al.*, 1990) and recrystallized from CH_3CN by slow diffusion of Et_2O to yield colourless crystals.

Refinement

H atoms bonded to C were inserted at calculated positions with C—H distances of 0.99 and 0.95 Å for saturated and unsaturated C atoms, respectively; they were refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms bonded to partial occupancy O atoms were not located or included in the model.

Figures

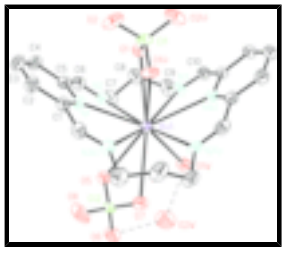

Fig. 1. Perspective view of complex (I); displacement ellipsoids are drawn at the 50% probability level and H-bonds are indicated by dashed lines. For clarity only one component of the disorder is shown and the H atoms are omitted. [Symmetry code (i) −*x*, *y*, −*z* + 3/2]

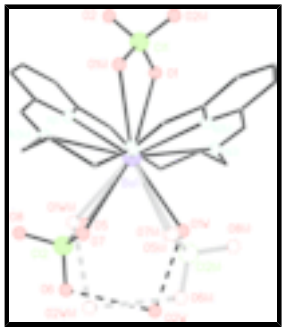

Fig. 2. Perspective view showing the two components of the disorder related by the 2-fold axis through Ba1 and Cl1 [Symmetry code (i) −*x*, *y*, −*z* + 3/2]. Dashed lines indicate H-bonds: O1W···O2W 2.761 (6) Å; O2W···O6 2.904 (5) Å.

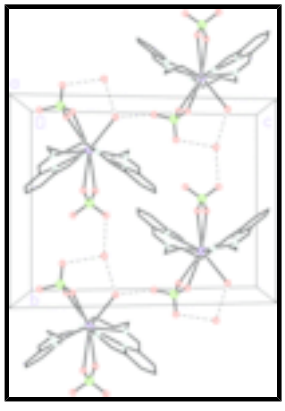

Fig. 3. Packing diagram viewed perpendicular to *a*, showing the two-dimensional H-bonded sheets. Only one component of the disorder is shown.

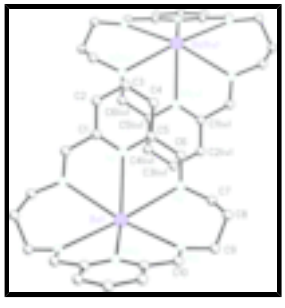

Fig. 4. The π-π stacking between pyridine diimine groups viewed perpendicular to the N1—C5 ring. H atoms and non-macrocyclic ligands omitted for clarity. [Symmetry code (iv) −*x* − 1/2, −*y* + 3/2, −*z* + 1]

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Crystal data

$[Ba(ClO_4)_2(C_{20}H_{22}N_6)(H_2O)]\cdot H_2O$	F_{000} = 1432
M_r = 718.71	D_x = 1.771 Mg m^{-3}

Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 9994 reflections
$a = 14.5247$ (8) Å	$\theta = 2.4$–31.7°
$b = 12.0634$ (6) Å	$\mu = 1.74$ mm^{-1}
$c = 15.8698$ (8) Å	$T = 150$ (2) K
$\beta = 104.157$ (1)°	Triangular prism, colourless
$V = 2696.2$ (2) Å^3	0.51 × 0.31 × 0.13 mm
$Z = 4$	

Data collection

Bruker APEXII diffractometer	4334 independent reflections
Radiation source: fine-focus sealed tube	4120 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 150$(2) K	$\theta_{max} = 31.9^\circ$
φ and ω scans	$\theta_{min} = 2.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -21 \rightarrow 21$
$T_{min} = 0.472$, $T_{max} = 0.806$	$k = -17 \rightarrow 17$
16000 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 4.1932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} = 0.002$
4334 reflections	$\Delta\rho_{max} = 0.69$ e Å^{-3}
213 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
3 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	0.788958 (11)	0.7500	0.01874 (4)	
N1	−0.10892 (11)	0.68917 (13)	0.59159 (10)	0.0238 (3)	
C1	−0.06707 (14)	0.65105 (15)	0.53091 (12)	0.0256 (3)	
C2	−0.11248 (16)	0.57923 (18)	0.46426 (13)	0.0338 (4)	
H2	−0.0805	0.5533	0.4225	0.041*	
C3	−0.20456 (17)	0.54690 (18)	0.46044 (15)	0.0381 (5)	
H3	−0.2369	0.4977	0.4163	0.046*	
C4	−0.24903 (15)	0.58707 (17)	0.52181 (15)	0.0352 (4)	
H4	−0.3127	0.5669	0.5200	0.042*	
C5	−0.19879 (13)	0.65772 (15)	0.58645 (13)	0.0267 (4)	
C6	−0.24753 (13)	0.70665 (17)	0.64921 (14)	0.0302 (4)	
H6	−0.3125	0.6892	0.6436	0.036*	
N2	−0.20673 (11)	0.77051 (14)	0.70992 (11)	0.0266 (3)	
C7	−0.26778 (15)	0.8175 (2)	0.76233 (14)	0.0356 (4)	0.90
H7A	−0.3350	0.8113	0.7297	0.043*	0.90
H7B	−0.2529	0.8972	0.7726	0.043*	0.90
C8	−0.25451 (17)	0.7586 (2)	0.84939 (17)	0.0383 (5)	0.90
H8A	−0.3117	0.7722	0.8714	0.046*	0.90
H8B	−0.2511	0.6779	0.8394	0.046*	0.90
C9	−0.16824 (16)	0.7917 (2)	0.91937 (15)	0.0407 (5)	0.90
H9A	−0.1659	0.8736	0.9230	0.049*	0.90
H9B	−0.1760	0.7636	0.9758	0.049*	0.90
C7'	−0.26778 (15)	0.8175 (2)	0.76233 (14)	0.0356 (4)	0.10
H7'1	−0.3091	0.7577	0.7752	0.043*	0.10
H7'2	−0.3095	0.8740	0.7270	0.043*	0.10
C8'	−0.2141 (14)	0.8725 (14)	0.8508 (9)	0.032 (4)*	0.10
H8'1	−0.1647	0.9230	0.8396	0.038*	0.10
H8'2	−0.2598	0.9178	0.8730	0.038*	0.10
C9'	−0.16824 (16)	0.7917 (2)	0.91937 (15)	0.0407 (5)	0.10
H9'1	−0.1576	0.8276	0.9770	0.049*	0.10
H9'2	−0.2113	0.7279	0.9185	0.049*	0.10
N3	−0.07714 (12)	0.75158 (15)	0.90665 (11)	0.0275 (3)	
C10	−0.02915 (14)	0.69174 (16)	0.96740 (12)	0.0280 (4)	
H10	−0.0564	0.6722	1.0140	0.034*	
Cl1	0.0000	0.48758 (5)	0.7500	0.02468 (12)	
O1	−0.07104 (10)	0.55775 (11)	0.77253 (10)	0.0303 (3)	
O2	−0.04305 (13)	0.41910 (14)	0.67689 (12)	0.0444 (4)	
Cl2	−0.00155 (6)	1.03329 (8)	0.62396 (6)	0.02486 (16)	0.50
O5	−0.0806 (3)	0.9790 (3)	0.6470 (2)	0.0381 (8)	0.50
O6	−0.0092 (3)	1.1495 (3)	0.6331 (2)	0.0408 (7)	0.50
O7	0.0840 (2)	0.9913 (3)	0.6816 (2)	0.0342 (6)	0.50
O8	−0.0029 (4)	1.0072 (4)	0.5355 (2)	0.0576 (11)	0.50

O1W	0.0299 (4)	0.9723 (3)	0.8653 (2)	0.0476 (10)	0.50
O2W	−0.0057 (4)	1.1901 (4)	0.8142 (3)	0.0690 (13)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.02017 (7)	0.01853 (7)	0.01998 (7)	0.000	0.00965 (5)	0.000
N1	0.0224 (7)	0.0224 (7)	0.0265 (7)	0.0014 (5)	0.0054 (5)	−0.0012 (5)
C1	0.0281 (8)	0.0230 (8)	0.0245 (8)	0.0044 (7)	0.0042 (7)	−0.0026 (6)
C2	0.0399 (11)	0.0295 (9)	0.0289 (9)	0.0056 (8)	0.0024 (8)	−0.0071 (7)
C3	0.0404 (11)	0.0286 (10)	0.0378 (11)	−0.0005 (8)	−0.0049 (9)	−0.0072 (8)
C4	0.0270 (9)	0.0284 (9)	0.0449 (12)	−0.0020 (8)	−0.0014 (8)	−0.0016 (8)
C5	0.0219 (8)	0.0226 (8)	0.0338 (9)	0.0016 (6)	0.0035 (7)	0.0016 (7)
C6	0.0186 (8)	0.0313 (9)	0.0411 (11)	0.0017 (7)	0.0083 (7)	0.0053 (8)
N2	0.0225 (7)	0.0299 (8)	0.0301 (8)	0.0078 (6)	0.0115 (6)	0.0064 (6)
C7	0.0272 (9)	0.0482 (12)	0.0351 (10)	0.0139 (9)	0.0151 (8)	0.0067 (9)
C8	0.0255 (10)	0.0550 (15)	0.0400 (12)	0.0071 (10)	0.0189 (9)	0.0136 (11)
C9	0.0325 (10)	0.0636 (15)	0.0322 (10)	0.0116 (10)	0.0201 (8)	0.0035 (10)
C7'	0.0272 (9)	0.0482 (12)	0.0351 (10)	0.0139 (9)	0.0151 (8)	0.0067 (9)
C9'	0.0325 (10)	0.0636 (15)	0.0322 (10)	0.0116 (10)	0.0201 (8)	0.0035 (10)
N3	0.0253 (7)	0.0348 (8)	0.0258 (7)	0.0016 (6)	0.0131 (6)	0.0015 (6)
C10	0.0307 (9)	0.0322 (9)	0.0235 (8)	−0.0059 (7)	0.0115 (7)	0.0018 (7)
Cl1	0.0260 (3)	0.0175 (2)	0.0348 (3)	0.000	0.0156 (2)	0.000
O1	0.0296 (7)	0.0251 (6)	0.0411 (8)	0.0065 (5)	0.0178 (6)	0.0012 (6)
O2	0.0469 (9)	0.0358 (8)	0.0572 (10)	−0.0167 (7)	0.0258 (8)	−0.0204 (8)
Cl2	0.0288 (4)	0.0247 (4)	0.0219 (4)	−0.0025 (3)	0.0077 (3)	0.0058 (3)
O5	0.0302 (16)	0.0428 (19)	0.0391 (18)	−0.0088 (14)	0.0041 (14)	0.0120 (14)
O6	0.059 (2)	0.0259 (15)	0.0359 (17)	0.0034 (14)	0.0078 (15)	0.0003 (13)
O7	0.0227 (13)	0.0346 (15)	0.0444 (17)	0.0007 (11)	0.0065 (12)	0.0083 (13)
O8	0.095 (3)	0.055 (2)	0.0287 (16)	0.011 (2)	0.0268 (19)	0.0088 (15)
O1W	0.091 (3)	0.0312 (18)	0.0255 (16)	−0.004 (2)	0.022 (2)	−0.0022 (13)
O2W	0.093 (4)	0.050 (2)	0.065 (3)	0.002 (2)	0.022 (3)	−0.003 (2)

Geometric parameters (Å, °)

Ba1—O1W	2.836 (4)	N2—C7	1.470 (2)
Ba1—N1	2.8856 (16)	C7—C8	1.523 (3)
Ba1—O5	2.893 (4)	C7—H7A	0.9900
Ba1—N2	2.9217 (16)	C7—H7B	0.9900
Ba1—N3	3.0002 (15)	C8—C9	1.511 (4)
Ba1—O1	3.0253 (14)	C8—H8A	0.9900
Ba1—O7	3.045 (3)	C8—H8B	0.9900
N1—C1	1.340 (2)	C9—N3	1.469 (3)
N1—C5	1.342 (2)	C9—H9A	0.9900
C1—C2	1.401 (3)	C9—H9B	0.9900
C1—C10^{i}	1.475 (3)	C8'—H8'1	0.9900
C2—C3	1.380 (3)	C8'—H8'2	0.9900
C2—H2	0.9500	N3—C10	1.268 (3)

C3—C4	1.381 (3)	C10—H10	0.9500
C3—H3	0.9500	Cl1—O2	1.4369 (17)
C4—C5	1.395 (3)	Cl1—O1	1.4455 (13)
C4—H4	0.9500	Cl2—O6	1.416 (3)
C5—C6	1.479 (3)	Cl2—O8	1.435 (3)
C6—N2	1.262 (3)	Cl2—O7	1.442 (3)
C6—H6	0.9500	Cl2—O5	1.444 (3)
O1W—Ba1—N1	148.48 (11)	N1—C1—C2	122.83 (19)
O1W—Ba1—N1^{i}	78.38 (9)	N1—C1—C10^{i}	117.85 (16)
N1—Ba1—N1^{i}	130.69 (6)	C2—C1—C10^{i}	119.24 (18)
O1W—Ba1—O5^{i}	16.22 (10)	C3—C2—C1	118.7 (2)
N1—Ba1—O5^{i}	152.02 (8)	C3—C2—H2	120.7
O1W—Ba1—O5	73.93 (10)	C1—C2—H2	120.7
N1—Ba1—O5	77.19 (8)	C2—C3—C4	119.02 (19)
N1^{i}—Ba1—O5	152.02 (8)	C2—C3—H3	120.5
O5^{i}—Ba1—O5	75.11 (15)	C4—C3—H3	120.5
O1W—Ba1—N2	100.79 (12)	C3—C4—C5	118.8 (2)
N1—Ba1—N2	57.54 (5)	C3—C4—H4	120.6
N1^{i}—Ba1—N2	118.24 (4)	C5—C4—H4	120.6
O5^{i}—Ba1—N2	115.84 (8)	N1—C5—C4	122.92 (19)
O5—Ba1—N2	71.63 (8)	N1—C5—C6	117.70 (17)
O1W—Ba1—N2^{i}	86.08 (12)	C4—C5—C6	119.26 (18)
N1—Ba1—N2^{i}	118.24 (4)	N2—C6—C5	123.03 (17)
O5—Ba1—N2^{i}	115.84 (8)	N2—C6—H6	118.5
N2—Ba1—N2^{i}	171.27 (6)	C5—C6—H6	118.5
O1W—Ba1—N3	67.18 (9)	C6—N2—C7	115.58 (18)
N1—Ba1—N3	115.02 (5)	C6—N2—Ba1	118.57 (12)
N1^{i}—Ba1—N3	56.75 (4)	C7—N2—Ba1	125.28 (13)
O5^{i}—Ba1—N3	80.34 (9)	N2—C7—C8	111.95 (18)
O5—Ba1—N3	113.95 (9)	N2—C7—H7A	109.2
N2—Ba1—N3	66.22 (5)	C8—C7—H7A	109.2
N2^{i}—Ba1—N3	112.35 (5)	N2—C7—H7B	109.2
O1W—Ba1—N3^{i}	128.49 (9)	C8—C7—H7B	109.2
N1—Ba1—N3^{i}	56.75 (4)	H7A—C7—H7B	107.9
O5—Ba1—N3^{i}	80.34 (9)	C9—C8—C7	116.2 (2)
N2—Ba1—N3^{i}	112.35 (5)	C9—C8—H8A	108.2
N3—Ba1—N3^{i}	162.71 (7)	C7—C8—H8A	108.2
O1W—Ba1—O1	130.24 (8)	C9—C8—H8B	108.2
N1—Ba1—O1	65.68 (4)	C7—C8—H8B	108.2
N1^{i}—Ba1—O1	69.06 (4)	H8A—C8—H8B	107.4
O5^{i}—Ba1—O1	140.06 (9)	N3—C9—C8	115.15 (19)
O5—Ba1—O1	134.03 (7)	N3—C9—H9A	108.5
N2—Ba1—O1	66.01 (4)	C8—C9—H9A	108.5
N2^{i}—Ba1—O1	105.43 (4)	N3—C9—H9B	108.5

N3—Ba1—O1	63.66 (4)	C8—C9—H9B	108.5
N3^{i}—Ba1—O1	99.59 (4)	H9A—C9—H9B	107.5
O1W—Ba1—O1^{i}	142.43 (10)	H8'1—C8'—H8'2	107.6
N1—Ba1—O1^{i}	69.06 (4)	C10—N3—C9	115.43 (17)
O5—Ba1—O1^{i}	140.06 (9)	C10—N3—Ba1	117.93 (12)
N2—Ba1—O1^{i}	105.43 (4)	C9—N3—Ba1	126.58 (13)
N3—Ba1—O1^{i}	99.59 (4)	N3—C10—C1^{i}	123.05 (17)
O1—Ba1—O1^{i}	45.57 (5)	N3—C10—H10	118.5
O1W—Ba1—O7^{i}	32.46 (13)	C1^{i}—C10—H10	118.5
O1W—Ba1—O7	65.97 (10)	O2—Cl1—O2^{i}	109.81 (16)
N1—Ba1—O7^{i}	117.57 (6)	O2—Cl1—O1	109.90 (10)
N1—Ba1—O7	101.89 (7)	O2^{i}—Cl1—O1	109.45 (9)
O5—Ba1—O7	45.97 (9)	O1^{i}—Cl1—O1	108.31 (12)
O5—Ba1—O7^{i}	54.82 (11)	Cl1—O1—Ba1	103.06 (7)
N2—Ba1—O7^{i}	70.05 (6)	O6—Cl2—O8	109.6 (2)
N2—Ba1—O7	117.60 (6)	O6—Cl2—O7	111.0 (2)
N3—Ba1—O7^{i}	64.02 (7)	O8—Cl2—O7	110.3 (2)
N3—Ba1—O7	132.77 (7)	O6—Cl2—O5	109.6 (2)
O1—Ba1—O7^{i}	121.28 (6)	O8—Cl2—O5	109.1 (3)
O1—Ba1—O7	163.58 (7)	O7—Cl2—O5	107.18 (19)
C1—N1—C5	117.70 (16)	Cl2—O5—Ba1	105.37 (18)
C1—N1—Ba1	121.39 (12)	Cl2—O7—Ba1	98.60 (14)
C5—N1—Ba1	119.25 (12)		

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

Table 1

Hydrogen-bond geometry (Å, °). The H atoms of these water molecules were not located.

D···A	D···A	D···A	D···A
O1W···O2W	2.761 (6)	O2W···O6	2.904 (7)
O1W···O8^{i}	2.866 (5)	O2W···O2^{ii}	2.846 (5)

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

Fig. 1

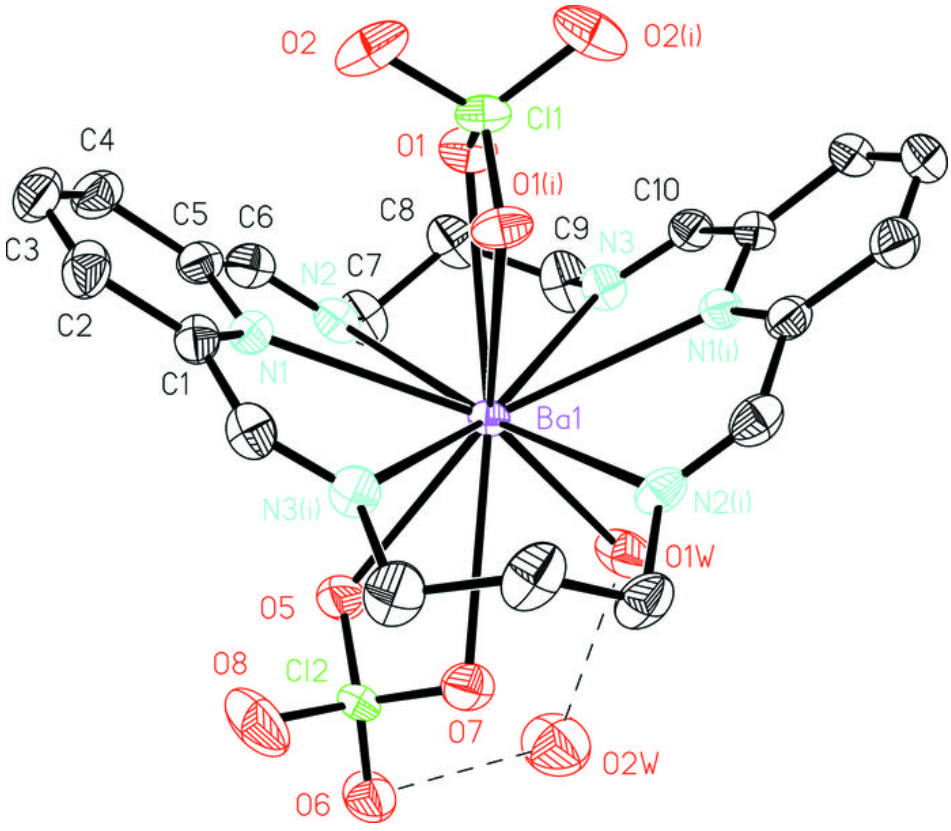

O2
O2(i)
Cl1
O1
O1(i)
C4
C5
C6
C8
C10
C9
N3
C3
N2
C7
C2
N1
N1(i)
C1
Ba1
N3(i)
N2(i)
O1W
O5
O8
Cl2
O7
O2W
O6

Fig. 2

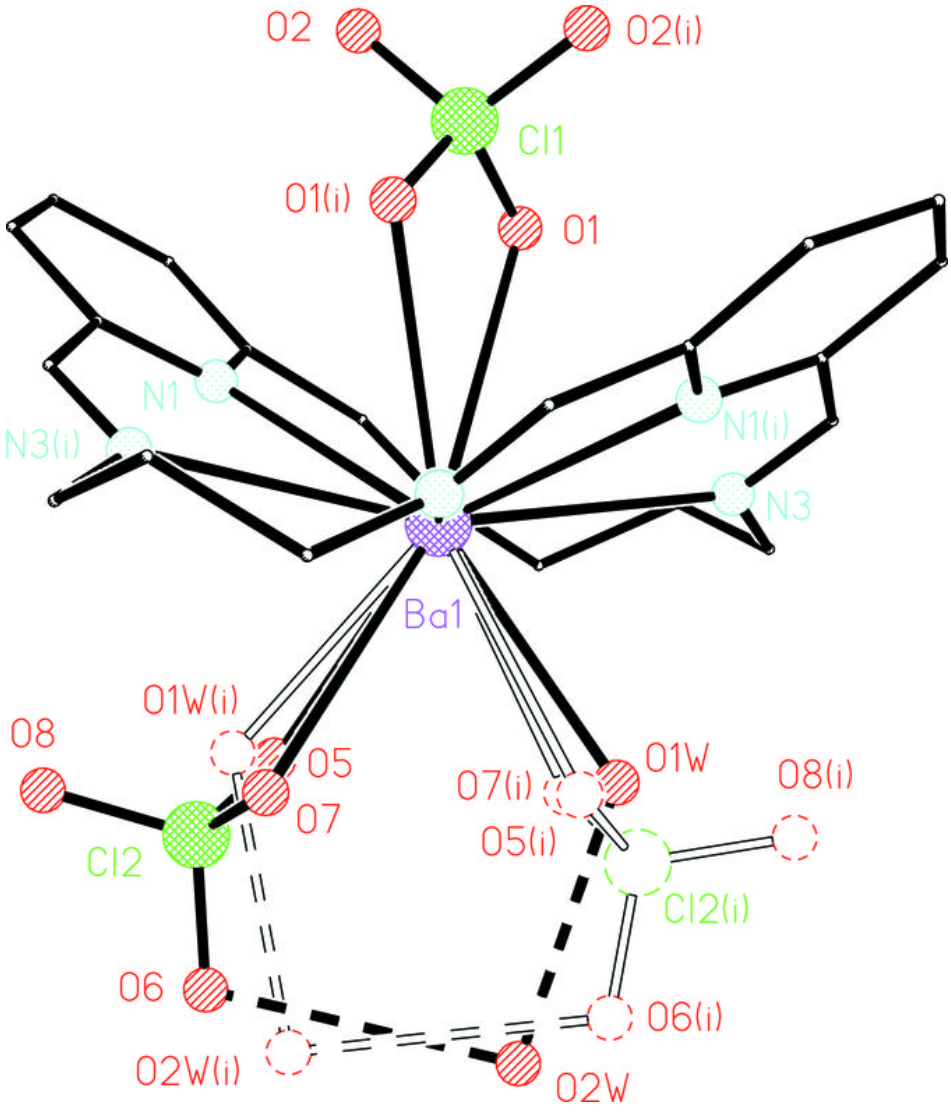

O2
O2(i)
Cl1
O1(i)
O1
N1
N3(i)
N1(i)
N3
Ba1
O1W(i)
O8
O5
O7
Cl2
O7(i)
O1W
O8(i)
O5(i)
Cl2(i)
O6
O6(i)
O2W(i)
O2W

Fig. 3

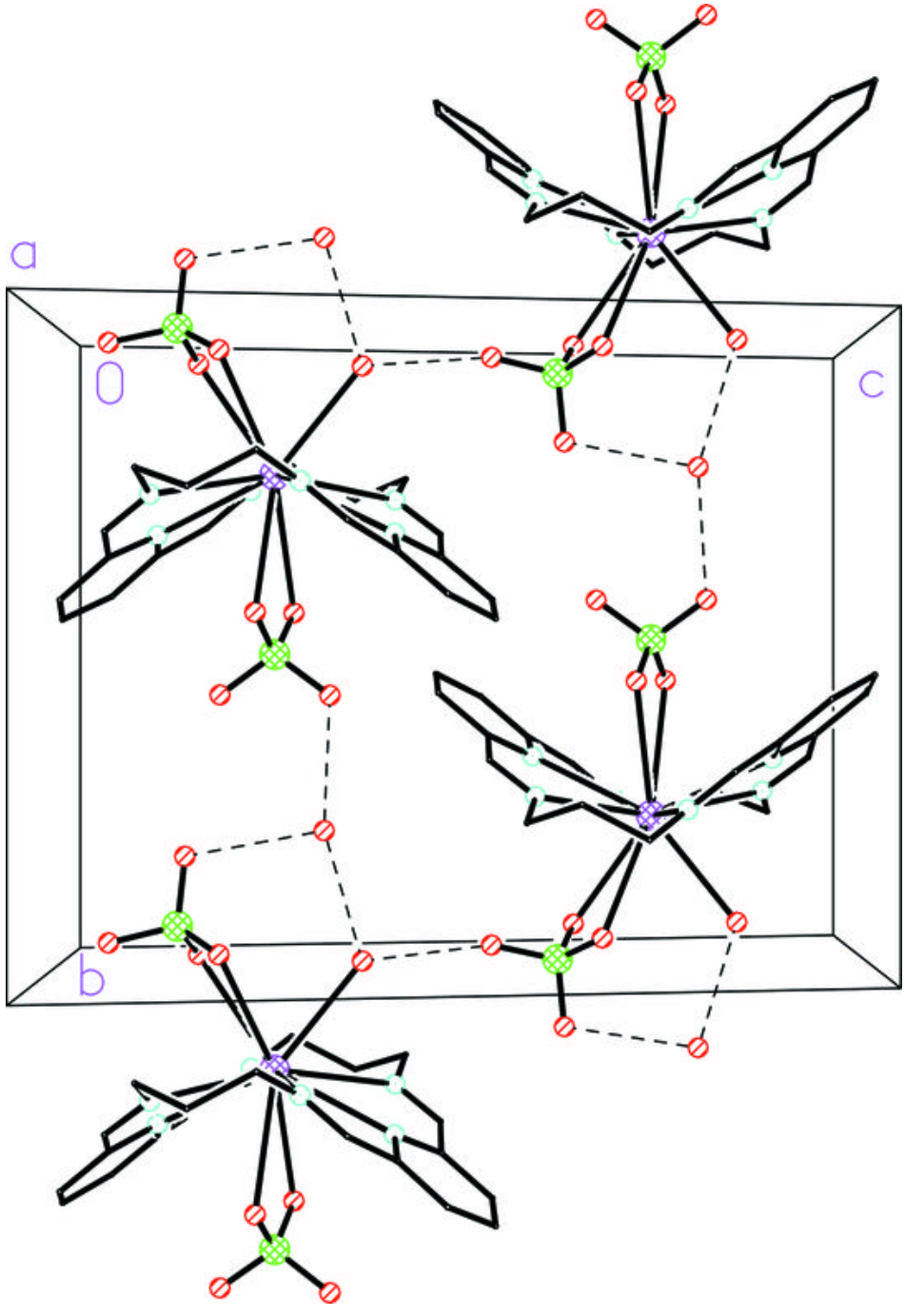
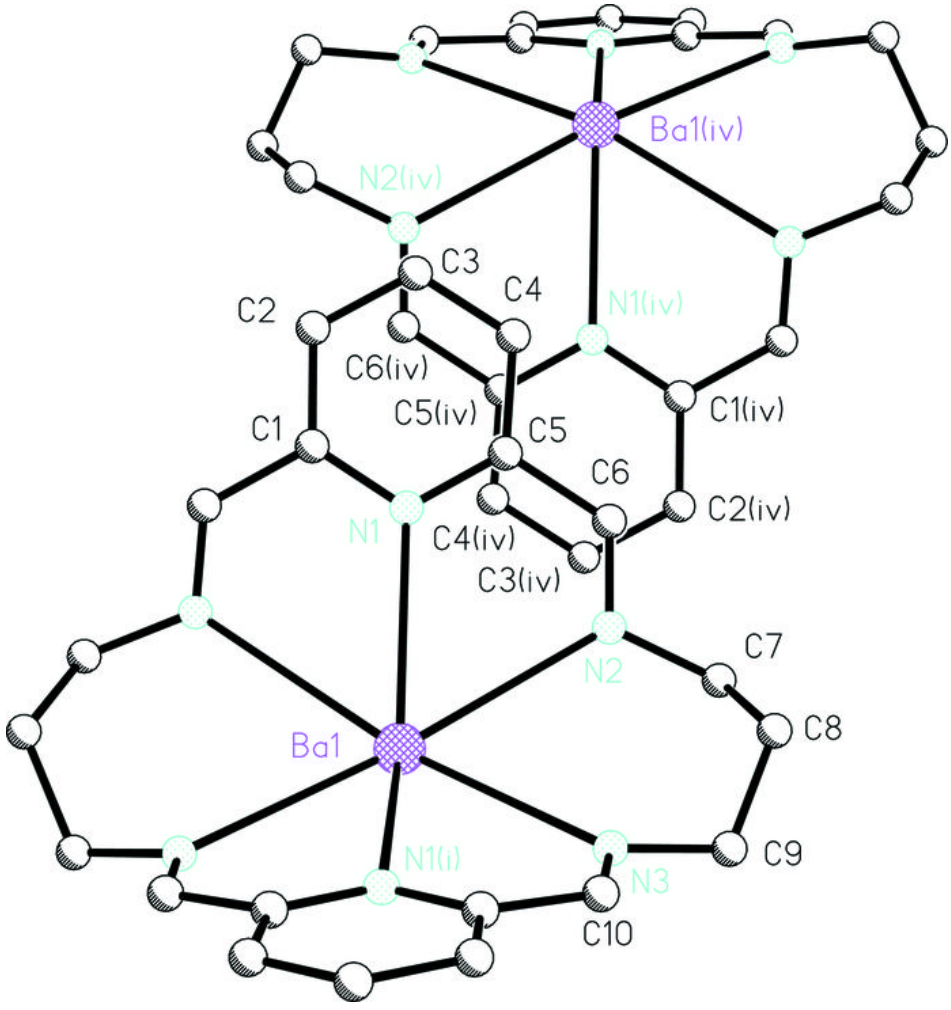


Fig. 4


Ba1(iv)
N2(iv)
C3
C4
N1(iv)
C2
C6(iv)
C5(iv)
C1(iv)
C1
C5
C6
C2(iv)
N1
C4(iv)
C3(iv)
C7
N2
C8
Ba1
N1(i)
N3
C9
C10