Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[tri-μ_2-aqua-(μ_3-pyridine-2,4-dicarboxylato-$\kappa^4N,O^2:O^2:O^{2'}$)barium]

Hoda Pasdar,[a]* Shadi Siabi,[a] Behrouz Notash,[b] Hossein Aghabozorg[a] and Naser Foroughifar[a]

[a]Department of Chemistry, North Tehran Branch, Islamic Azad University, Tehran, Iran, and [b]Department of Chemistry, Shahid Beheshti University, G. C. Evin, Tehran 1983963113, Iran
Correspondence e-mail: h_pasdar@iau-tnb.ac.ir

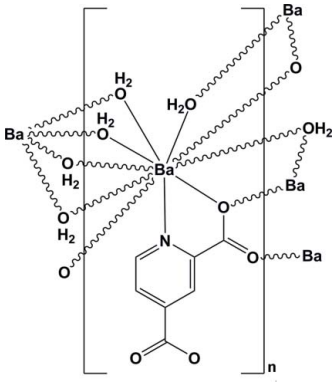
Received 9 May 2011; accepted 26 May 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.057; data-to-parameter ratio = 15.8.

In the polymeric title compound, $[Ba(C_7H_3NO_4)(H_2O)_3]_n$, the Ba^{II} ion is ten-coordinated in an NO_9 environment by one N atom and three O atoms from three pyridine-2,4-dicarboxylate (pydc) ligands and six water molecules. The μ_3-pydc ligands and the bridging water molecules connect the Ba atoms into a layer parallel to (100). The crystal packing is stabilized by O—H···O and C—H···O hydrogen bonds.

Related literature

For related compounds with pyridine dicarboxylic acid derivatives, see: Aghabozorg *et al.* (2008, 2011*a*,*b*,*c*,*d*); Noro *et al.* (2005); Pasdar *et al.* (2011*a*,*b*); Wang *et al.* (2007).



Experimental

Crystal data

$[Ba(C_7H_3NO_4)(H_2O)_3]$
M_r = 356.48
Monoclinic, $P2_1/c$
a = 11.079 (2) Å
b = 13.714 (3) Å
c = 6.5961 (13) Å
β = 94.13 (3)°
V = 999.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.00 mm^{-1}
T = 298 K
0.39 × 0.38 × 0.33 mm

Data collection

Stoe IPDS-2T diffractometer
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
T_{min} = 0.410, T_{max} = 0.460
7321 measured reflections
2681 independent reflections
2515 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.057
S = 1.10
2681 reflections
170 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.48	3.161 (3)	130
O5—H5A···O1^{ii}	0.77 (5)	2.14 (4)	2.881 (3)	162 (4)
O5—H5B···O4^{iii}	0.77 (5)	2.02 (5)	2.785 (3)	174 (4)
O6—H6A···O4^{iv}	0.91 (4)	2.03 (4)	2.865 (3)	151 (3)
O6—H6B···O3^{v}	0.76 (4)	2.08 (4)	2.816 (3)	167 (4)
O7—H7A···O3^{v}	0.85 (5)	1.96 (5)	2.809 (3)	175 (4)
O7—H7B···O4^{vi}	0.75 (4)	2.11 (4)	2.810 (3)	155 (4)

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge the Islamic Azad University, North Tehran Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2431).

References

Aghabozorg, H., Bayan, M., Mirzaei, M. & Notash, B. (2011*a*). *Acta Cryst.* E**67**, o610.
Aghabozorg, H., Goodarzi, S., Mirzaei, M. & Notash, B. (2011*b*). *Acta Cryst.* E**67**, m290.
Aghabozorg, H., Jafarbak, F., Mirzaei, M. & Notash, B. (2011*c*). *Acta Cryst.* E**67**, m435–m436.
Aghabozorg, H., Manteghi, F. & Sheshmani, S. (2008). *J. Iran. Chem. Soc.* **5**, 184–227.
Aghabozorg, H., Saemi, M., Khazaei, Z., Amani, V. & Notash, B. (2011*d*). *Acta Cryst.* E**67**, o292.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Noro, S.-L., Miyasaka, H., Kitagawa, S., Wada, T., Okubo, T., Yamashita, M. & Mitani, T. (2005). *Inorg. Chem.* **44**, 133–146.
Pasdar, H., Sadat Kashani, S., Aghabozorg, H. & Notash, B. (2011*a*). *Acta Cryst.* E**67**, m193–m194.
Pasdar, H., Safari, Z., Aghabozorg, H., Notash, B. & Mirzaei, M. (2011*b*). *Acta Cryst.* E**67**, m221.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2005). *X-AREA*, *X-SHAPE* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.
Wang, L.-B., Pan, Y.-R., Zhan, P.-Y., Niu, Y.-L. & Zhang, G.-Q. (2007). *Acta Cryst.* E**63**, m204–m206.

supplementary materials

Acta Cryst. (2011). E**67**, m848 [**doi:10.1107/S1600536811020204**]

Poly[tri-μ_2-aqua-(μ_3-pyridine-2,4-dicarboxylato-$\kappa^4N,O^2:O^2:O^{2'}$)barium]

H. Pasdar, S. Siabi, B. Notash, H. Aghabozorg and N. Foroughifar

Comment

Pyridine dicarboxylic acid derivatives, depending on the composition and situation of carboxylic groups and the number of deprotonated carboxylic groups, can form wide variety of compounds from organic proton transfer compounds (Aghabozorg *et al.*, 2011*a*,*c*,*d*) to discrete coordination compounds (Aghabozorg *et al.*, 2008, 2011*b*; Noro *et al.*, 2005; Pasdar *et al.*, 2011*a*) and coordination polymers (Pasdar *et al.*, 2011*b*).

The asymmetric unit of the title compound is shown in Fig. 1. Two carboxylate groups of the pyridine-2,4-dicarboxylate (pydc) ligand are deprotonated and Ba^{II} ion is ten-coordinated in an NO_9 environment (Fig. 2). The crystal structure shows that the compound is a two-dimensional polymer (Fig. 3). O—H···O and C—H···O hydrogen bonds stabilize the crystal packing (Table 1).

Experimental

A mixture of $Ba(NO_3)_2$ (0.132 g), pyridine-2,4-dicarboxylic acid (0.085 g), 2,2'-bipyridine (0.156 g) in H_2O (60 ml) was stirred at 40°C for 1 h. The solution was filtered, and the filtrate was stand at room temperature. After two weaks, colorless block-shaped crystals of the title compound were obtained.

Refinement

H atoms of water molecules were found in a difference Fourier map and refined isotropically. H6B was refined with a distance restraint of O—H = 0.75 (3). C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron density was found at 0.80 Å from Ba1 atom and the deepest hole at 0.80 Å from Ba1 atom.

Figures

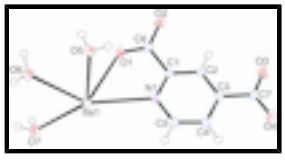


Fig. 1. The asymmetric unit of the title compound, with displacement ellipsoids drawn at 50% probability level.

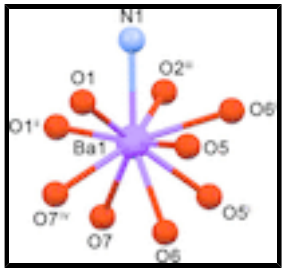


Fig. 2. The coordination environment around Ba^{II} ion in the title compound. [Symmetry codes: (i) -*x*, -*y*+1, -*z*; (ii) *x*, -*y*+3/2, *z*-1/2; (iii) *x*, *y*, *z*-1; (iv) *x*, -*y*+3/2, *z*+1/2.]

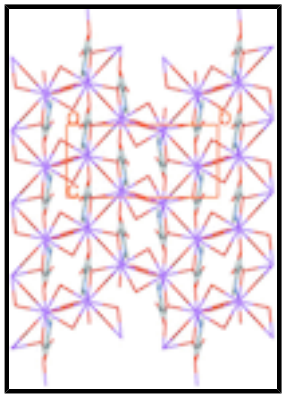


Fig. 3. A view of the two-dimensional structure of the title compound viewed down the *a* axis. H atoms have been omitted for clarity.

Poly[tri-μ$_2$-aqua-(μ$_3$-pyridine-2,4-dicarboxylato- $\kappa^4N,O^2:O^2:O^{2'}$)barium]

Crystal data

$[Ba(C_7H_3NO_4)(H_2O)_3]$	$F(000) = 680$
$M_r = 356.48$	$D_x = 2.369$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2681 reflections
$a = 11.079$ (2) Å	$\theta = 2.4$–$29.1°$
$b = 13.714$ (3) Å	$\mu = 4.00$ mm^{-1}
$c = 6.5961$ (13) Å	$T = 298$ K
$\beta = 94.13$ (3)°	Block, colorless
$V = 999.6$ (3) Å^3	0.39 × 0.38 × 0.33 mm
$Z = 4$	

Data collection

Stoe IPDS-2T diffractometer	2681 independent reflections
Radiation source: fine-focus sealed tube	2515 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.041$
ω scans	$\theta_{max} = 29.1°$, $\theta_{min} = 2.4°$
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)	$h = -15 \rightarrow 13$
$T_{min} = 0.410$, $T_{max} = 0.460$	$k = -18 \rightarrow 18$
7321 measured reflections	$l = -9 \rightarrow 9$

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 atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.2871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.002$
2681 reflections	$\Delta\rho_{max} = 2.20$ e Å^{-3}
170 parameters	$\Delta\rho_{min} = -0.60$ e Å^{-3}
1 restraint	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0182 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
H6B	−0.211 (3)	0.577 (3)	−0.019 (6)	0.045 (11)*
O6	−0.16582 (16)	0.54989 (14)	0.0517 (3)	0.0245 (3)
O7	−0.09028 (16)	0.75423 (14)	−0.1846 (3)	0.0234 (3)
O5	0.02949 (17)	0.45857 (14)	0.2957 (3)	0.0233 (3)
Ba1	0.074526 (10)	0.638147 (8)	0.073630 (17)	0.01506 (7)
C2	0.4566 (2)	0.63768 (15)	0.5688 (4)	0.0179 (4)
H2	0.4672	0.6508	0.7073	0.021*
N1	0.32012 (18)	0.61649 (17)	0.2709 (3)	0.0223 (4)
C1	0.3411 (2)	0.63417 (14)	0.4713 (4)	0.0166 (4)
C5	0.4167 (2)	0.6023 (2)	0.1646 (4)	0.0290 (5)
H5	0.4040	0.5907	0.0258	0.035*
O1	0.13032 (15)	0.66224 (14)	0.4870 (3)	0.0227 (3)
O2	0.24279 (19)	0.65068 (17)	0.7766 (3)	0.0341 (5)
C6	0.2301 (2)	0.64984 (16)	0.5894 (4)	0.0175 (4)
C7	0.6829 (2)	0.62030 (18)	0.5578 (4)	0.0206 (4)
C3	0.5562 (2)	0.62132 (17)	0.4560 (4)	0.0186 (4)
C4	0.5348 (2)	0.6037 (2)	0.2492 (4)	0.0268 (5)
H4	0.5990	0.5930	0.1685	0.032*
O3	0.69566 (19)	0.64657 (16)	0.7382 (3)	0.0340 (5)
O4	0.76764 (15)	0.59321 (15)	0.4537 (3)	0.0278 (4)
H5A	−0.019 (4)	0.438 (3)	0.361 (6)	0.047 (11)*
H5B	0.087 (4)	0.448 (3)	0.364 (6)	0.048 (12)*
H7B	−0.116 (4)	0.792 (3)	−0.116 (6)	0.039 (10)*
H6A	−0.209 (4)	0.550 (3)	0.164 (6)	0.043 (10)*
H7A	−0.155 (4)	0.723 (3)	−0.215 (7)	0.060 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O6	0.0208 (8)	0.0317 (9)	0.0211 (8)	0.0043 (7)	0.0026 (7)	0.0017 (7)
O7	0.0204 (8)	0.0251 (8)	0.0246 (8)	−0.0010 (7)	0.0016 (7)	−0.0014 (7)
O5	0.0192 (8)	0.0316 (9)	0.0191 (8)	0.0005 (7)	0.0014 (7)	0.0040 (7)
Ba1	0.01347 (9)	0.01844 (9)	0.01335 (10)	0.00009 (4)	0.00141 (5)	−0.00001 (4)
C2	0.0153 (10)	0.0255 (11)	0.0128 (10)	−0.0002 (7)	0.0004 (8)	0.0007 (7)
N1	0.0169 (9)	0.0350 (10)	0.0148 (9)	0.0023 (8)	−0.0012 (7)	−0.0034 (8)
C1	0.0128 (9)	0.0217 (10)	0.0156 (10)	0.0007 (7)	0.0026 (8)	0.0003 (7)
C5	0.0177 (10)	0.0535 (16)	0.0157 (10)	0.0048 (11)	0.0003 (8)	−0.0053 (11)
O1	0.0135 (7)	0.0330 (8)	0.0218 (8)	0.0041 (6)	0.0017 (6)	0.0010 (7)
O2	0.0216 (9)	0.0644 (14)	0.0170 (9)	−0.0006 (8)	0.0052 (7)	−0.0048 (8)
C6	0.0138 (9)	0.0202 (9)	0.0189 (10)	−0.0006 (7)	0.0042 (8)	−0.0010 (8)
C7	0.0137 (9)	0.0240 (9)	0.0237 (11)	−0.0005 (8)	−0.0013 (8)	0.0044 (9)
C3	0.0146 (9)	0.0227 (9)	0.0182 (10)	0.0006 (8)	0.0002 (8)	0.0014 (8)
C4	0.0160 (10)	0.0466 (15)	0.0179 (11)	0.0017 (10)	0.0026 (8)	−0.0032 (10)
O3	0.0237 (10)	0.0518 (12)	0.0252 (10)	0.0041 (8)	−0.0065 (8)	−0.0064 (8)
O4	0.0156 (7)	0.0406 (10)	0.0272 (9)	0.0030 (7)	0.0023 (6)	0.0028 (8)

Geometric parameters (Å, °)

O6—H6B	0.75 (3)	C2—C1	1.391 (3)
O6—H6A	0.91 (4)	C2—C3	1.393 (3)
O7—H7B	0.75 (4)	C2—H2	0.9300
O7—H7A	0.85 (5)	N1—C5	1.336 (3)
O5—H5A	0.77 (5)	N1—C1	1.347 (3)
O5—H5B	0.77 (5)	C1—C6	1.518 (3)
Ba1—O1	2.7720 (19)	C5—C4	1.385 (3)
Ba1—O2^{i}	2.805 (2)	C5—H5	0.9300
Ba1—O1^{ii}	2.8728 (19)	O1—C6	1.265 (3)
Ba1—O7^{iii}	2.9111 (18)	O2—C6	1.233 (3)
Ba1—O7	2.8846 (19)	C7—O3	1.242 (3)
Ba1—O6^{iv}	2.9115 (19)	C7—O4	1.258 (3)
Ba1—O5^{iv}	2.935 (2)	C7—C3	1.511 (3)
Ba1—O5	2.9263 (19)	C3—C4	1.389 (3)
Ba1—N1	2.945 (2)	C4—H4	0.9300
Ba1—O6	2.9190 (19)		
Ba1^{iv}—O6—Ba1	92.69 (5)	O7—Ba1—N1	147.33 (6)
Ba1^{iv}—O6—H6B	119 (3)	O7^{iii}—Ba1—N1	113.88 (6)
Ba1—O6—H6B	113 (3)	O6^{iv}—Ba1—N1	72.99 (6)
Ba1^{iv}—O6—H6A	117 (2)	O6—Ba1—N1	142.22 (6)
Ba1—O6—H6A	119 (2)	O5—Ba1—N1	83.07 (6)
H6B—O6—H6A	98 (4)	O5^{iv}—Ba1—N1	128.03 (6)
Ba1—O7—Ba1^{ii}	102.01 (6)	O1—Ba1—C6^{ii}	77.88 (6)

Ba1—O7—H7B	106 (3)	O2^{i}—Ba1—C6^{ii}	66.76 (6)
Ba1^{ii}—O7—H7B	105 (3)	O1^{ii}—Ba1—C6^{ii}	21.45 (5)
Ba1—O7—H7A	110 (3)	O7—Ba1—C6^{ii}	80.97 (6)
Ba1^{ii}—O7—H7A	133 (3)	O7^{iii}—Ba1—C6^{ii}	83.42 (5)
H7B—O7—H7A	98 (4)	O6^{iv}—Ba1—C6^{ii}	125.75 (5)
Ba1—O5—Ba1^{iv}	92.06 (5)	O6—Ba1—C6^{ii}	145.09 (5)
Ba1—O5—H5A	138 (3)	O5—Ba1—C6^{ii}	144.49 (6)
Ba1^{iv}—O5—H5A	93 (3)	O5^{iv}—Ba1—C6^{ii}	125.70 (5)
Ba1—O5—H5B	107 (3)	N1—Ba1—C6^{ii}	67.67 (6)
Ba1^{iv}—O5—H5B	131 (3)	O1—Ba1—Ba1^{iv}	112.92 (4)
H5A—O5—H5B	101 (4)	O2^{i}—Ba1—Ba1^{iv}	99.38 (5)
O1—Ba1—O2^{i}	124.57 (6)	O1^{ii}—Ba1—Ba1^{iv}	153.68 (4)
O1—Ba1—O1^{ii}	92.64 (5)	O7—Ba1—Ba1^{iv}	98.00 (4)
O2^{i}—Ba1—O1^{ii}	68.86 (6)	O7^{iii}—Ba1—Ba1^{iv}	109.33 (4)
O1—Ba1—O7	127.00 (5)	O6^{iv}—Ba1—Ba1^{iv}	43.72 (4)
O2^{i}—Ba1—O7	88.74 (6)	O6—Ba1—Ba1^{iv}	43.58 (4)
O1^{ii}—Ba1—O7	59.52 (5)	O5—Ba1—Ba1^{iv}	44.06 (4)
O1—Ba1—O7^{iii}	60.32 (5)	O5^{iv}—Ba1—Ba1^{iv}	43.89 (4)
O2^{i}—Ba1—O7^{iii}	145.70 (6)	N1—Ba1—Ba1^{iv}	110.18 (5)
O1^{ii}—Ba1—O7^{iii}	77.19 (5)	C1—C2—C3	119.0 (2)
O7—Ba1—O7^{iii}	69.42 (3)	C1—C2—H2	120.5
O1—Ba1—O6^{iv}	109.12 (5)	C3—C2—H2	120.5
O2^{i}—Ba1—O6^{iv}	66.05 (6)	C5—N1—C1	116.9 (2)
O1^{ii}—Ba1—O6^{iv}	134.70 (5)	C5—N1—Ba1	122.17 (16)
O7—Ba1—O6^{iv}	122.63 (6)	C1—N1—Ba1	120.28 (14)
O7^{iii}—Ba1—O6^{iv}	148.11 (5)	N1—C1—C2	123.3 (2)
O1—Ba1—O6	103.66 (6)	N1—C1—C6	116.1 (2)
O2^{i}—Ba1—O6	129.84 (6)	C2—C1—C6	120.7 (2)
O1^{ii}—Ba1—O6	126.43 (5)	N1—C5—C4	123.8 (2)
O7—Ba1—O6	70.32 (5)	N1—C5—H5	118.1
O7^{iii}—Ba1—O6	68.38 (5)	C4—C5—H5	118.1
O6^{iv}—Ba1—O6	87.31 (5)	C6—O1—Ba1	129.32 (14)
O1—Ba1—O5	69.02 (5)	C6—O1—Ba1^{iii}	102.37 (14)
O2^{i}—Ba1—O5	123.15 (6)	Ba1—O1—Ba1^{iii}	105.86 (6)
O1^{ii}—Ba1—O5	161.49 (5)	C6—O2—Ba1^{v}	131.70 (16)
O7—Ba1—O5	129.53 (5)	O2—C6—O1	124.5 (2)
O7^{iii}—Ba1—O5	90.93 (5)	O2—C6—C1	118.5 (2)
O6^{iv}—Ba1—O5	58.13 (5)	O1—C6—C1	117.0 (2)
O6—Ba1—O5	59.20 (6)	O2—C6—Ba1^{iii}	92.52 (15)
O1—Ba1—O5^{iv}	156.43 (5)	O1—C6—Ba1^{iii}	56.18 (12)
O2^{i}—Ba1—O5^{iv}	71.89 (6)	C1—C6—Ba1^{iii}	122.45 (13)

O1^{ii}—Ba1—O5^{iv}	110.05 (5)	O3—C7—O4	124.8 (2)
O7—Ba1—O5^{iv}	64.24 (6)	O3—C7—C3	117.5 (2)
O7^{iii}—Ba1—O5^{iv}	117.35 (5)	O4—C7—C3	117.8 (2)
O6^{iv}—Ba1—O5^{iv}	59.19 (5)	C4—C3—C2	117.8 (2)
O6—Ba1—O5^{iv}	57.95 (5)	C4—C3—C7	121.5 (2)
O5—Ba1—O5^{iv}	87.94 (5)	C2—C3—C7	120.7 (2)
O1—Ba1—N1	56.21 (6)	C5—C4—C3	119.2 (2)
O2^{i}—Ba1—N1	71.07 (6)	C5—C4—H4	120.4
O1^{ii}—Ba1—N1	88.79 (6)	C3—C4—H4	120.4
Ba1^{ii}—O7—Ba1—O1	108.60 (7)	C5—N1—C1—C2	−0.2 (4)
Ba1^{ii}—O7—Ba1—O2^{i}	−25.36 (7)	Ba1—N1—C1—C2	−171.43 (15)
Ba1^{ii}—O7—Ba1—O1^{ii}	40.72 (5)	C5—N1—C1—C6	−179.8 (2)
Ba1^{ii}—O7—Ba1—O7^{iii}	127.63 (8)	Ba1—N1—C1—C6	9.0 (3)
Ba1^{ii}—O7—Ba1—O6^{iv}	−85.61 (7)	C3—C2—C1—N1	−0.6 (3)
Ba1^{ii}—O7—Ba1—O6	−158.86 (7)	C3—C2—C1—C6	178.93 (19)
Ba1^{ii}—O7—Ba1—O5	−159.07 (5)	C1—N1—C5—C4	0.7 (4)
Ba1^{ii}—O7—Ba1—O5^{iv}	−95.80 (7)	Ba1—N1—C5—C4	171.8 (2)
Ba1^{ii}—O7—Ba1—N1	25.18 (13)	O2^{i}—Ba1—O1—C6	−24.9 (2)
Ba1^{ii}—O7—Ba1—C6^{ii}	41.31 (6)	O1^{ii}—Ba1—O1—C6	−90.95 (18)
Ba1^{ii}—O7—Ba1—Ba1^{iv}	−124.66 (5)	O7—Ba1—O1—C6	−144.00 (18)
Ba1^{iv}—O6—Ba1—O1	−109.03 (5)	O7^{iii}—Ba1—O1—C6	−164.6 (2)
Ba1^{iv}—O6—Ba1—O2^{i}	55.35 (9)	O6^{iv}—Ba1—O1—C6	48.6 (2)
Ba1^{iv}—O6—Ba1—O1^{ii}	147.19 (5)	O6—Ba1—O1—C6	140.52 (19)
Ba1^{iv}—O6—Ba1—O7	126.16 (6)	O5—Ba1—O1—C6	91.6 (2)
Ba1^{iv}—O6—Ba1—O7^{iii}	−158.90 (7)	O5^{iv}—Ba1—O1—C6	104.5 (2)
Ba1^{iv}—O6—Ba1—O6^{iv}	0.0	N1—Ba1—O1—C6	−4.18 (18)
Ba1^{iv}—O6—Ba1—O5	−54.04 (5)	C6^{ii}—Ba1—O1—C6	−75.3 (2)
Ba1^{iv}—O6—Ba1—O5^{iv}	54.86 (5)	Ba1^{iv}—Ba1—O1—C6	95.48 (19)
Ba1^{iv}—O6—Ba1—N1	−57.40 (10)	O2^{i}—Ba1—O1—Ba1^{iii}	96.43 (7)
Ba1^{iv}—O6—Ba1—C6^{ii}	162.67 (7)	O1^{ii}—Ba1—O1—Ba1^{iii}	30.42 (8)
Ba1^{iv}—O5—Ba1—O1	174.89 (6)	O7—Ba1—O1—Ba1^{iii}	−22.64 (8)
Ba1^{iv}—O5—Ba1—O2^{i}	−66.73 (8)	O7^{iii}—Ba1—O1—Ba1^{iii}	−43.21 (5)
Ba1^{iv}—O5—Ba1—O1^{ii}	166.78 (13)	O6^{iv}—Ba1—O1—Ba1^{iii}	170.00 (5)
Ba1^{iv}—O5—Ba1—O7	53.60 (8)	O6—Ba1—O1—Ba1^{iii}	−98.11 (6)
Ba1^{iv}—O5—Ba1—O7^{iii}	117.34 (5)	O5—Ba1—O1—Ba1^{iii}	−147.01 (7)
Ba1^{iv}—O5—Ba1—O6^{iv}	−54.46 (5)	O5^{iv}—Ba1—O1—Ba1^{iii}	−134.14 (11)
Ba1^{iv}—O5—Ba1—O6	53.36 (6)	N1—Ba1—O1—Ba1^{iii}	117.19 (8)
Ba1^{iv}—O5—Ba1—O5^{iv}	0.0	C6^{ii}—Ba1—O1—Ba1^{iii}	46.08 (6)
Ba1^{iv}—O5—Ba1—N1	−128.71 (6)	Ba1^{iv}—Ba1—O1—Ba1^{iii}	−143.15 (4)
Ba1^{iv}—O5—Ba1—C6^{ii}	−162.71 (6)	Ba1^{v}—O2—C6—O1	14.9 (4)
O1—Ba1—N1—C5	−174.1 (2)	Ba1^{v}—O2—C6—C1	−165.84 (15)

O2^{i}—Ba1—N1—C5	−12.0 (2)	Ba1^{v}—O2—C6—Ba1^{iii}	64.7 (2)
O1^{ii}—Ba1—N1—C5	−80.1 (2)	Ba1—O1—C6—O2	−170.54 (18)
O7—Ba1—N1—C5	−66.7 (3)	Ba1^{iii}—O1—C6—O2	66.7 (3)
O7^{iii}—Ba1—N1—C5	−155.5 (2)	Ba1—O1—C6—C1	10.2 (3)
O6^{iv}—Ba1—N1—C5	57.8 (2)	Ba1^{iii}—O1—C6—C1	−112.54 (17)
O6—Ba1—N1—C5	119.5 (2)	Ba1—O1—C6—Ba1^{iii}	122.77 (18)
O5—Ba1—N1—C5	116.6 (2)	N1—C1—C6—O2	168.6 (2)
O5^{iv}—Ba1—N1—C5	34.7 (2)	C2—C1—C6—O2	−11.0 (3)
C6^{ii}—Ba1—N1—C5	−84.0 (2)	N1—C1—C6—O1	−12.2 (3)
Ba1^{iv}—Ba1—N1—C5	81.3 (2)	C2—C1—C6—O1	168.2 (2)
O1—Ba1—N1—C1	−3.35 (16)	N1—C1—C6—Ba1^{iii}	−77.6 (2)
O2^{i}—Ba1—N1—C1	158.68 (19)	C2—C1—C6—Ba1^{iii}	102.8 (2)
O1^{ii}—Ba1—N1—C1	90.65 (18)	C1—C2—C3—C4	1.0 (3)
O7—Ba1—N1—C1	103.99 (18)	C1—C2—C3—C7	−177.42 (19)
O7^{iii}—Ba1—N1—C1	15.24 (19)	O3—C7—C3—C4	172.7 (3)
O6^{iv}—Ba1—N1—C1	−131.43 (19)	O4—C7—C3—C4	−7.1 (4)
O6—Ba1—N1—C1	−69.8 (2)	O3—C7—C3—C2	−8.9 (3)
O5—Ba1—N1—C1	−72.70 (18)	O4—C7—C3—C2	171.3 (2)
O5^{iv}—Ba1—N1—C1	−154.60 (16)	N1—C5—C4—C3	−0.4 (5)
C6^{ii}—Ba1—N1—C1	86.74 (18)	C2—C3—C4—C5	−0.5 (4)
Ba1^{iv}—Ba1—N1—C1	−108.02 (17)	C7—C3—C4—C5	177.9 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.48	3.161 (3)	130
O5—H5A···O1^{vi}	0.77 (5)	2.14 (4)	2.881 (3)	162 (4)
O5—H5B···O4^{vii}	0.77 (5)	2.02 (5)	2.785 (3)	174 (4)
O6—H6A···O4^{viii}	0.91 (4)	2.03 (4)	2.865 (3)	151 (3)
O6—H6B···O3^{ix}	0.76 (4)	2.08 (4)	2.816 (3)	167 (4)
O7—H7A···O3^{ix}	0.85 (5)	1.96 (5)	2.809 (3)	175 (4)
O7—H7B···O4^{x}	0.75 (4)	2.11 (4)	2.810 (3)	155 (4)

Symmetry codes: (i) *x*, *y*, *z*−1; (vi) −*x*, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) *x*−1, *y*, *z*; (ix) *x*−1, *y*, *z*−1; (x) *x*−1, −*y*+3/2, *z*−1/2.

Fig. 1

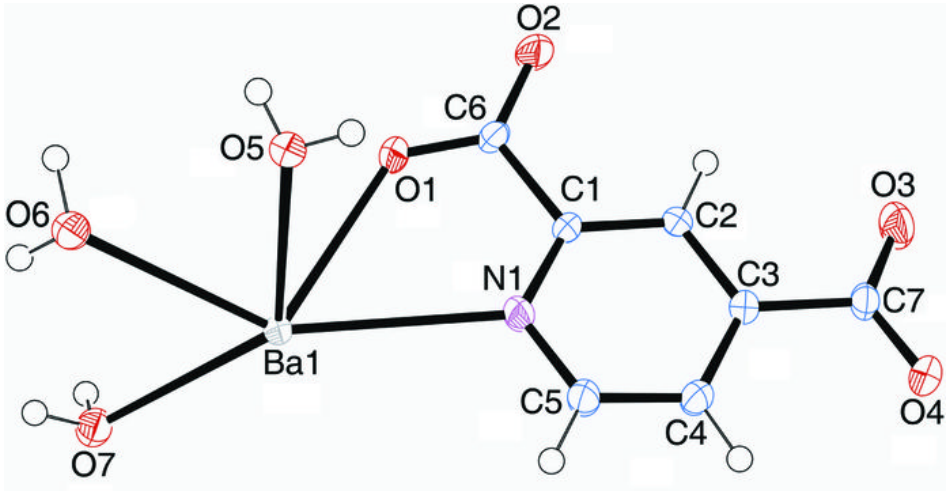


Fig. 2

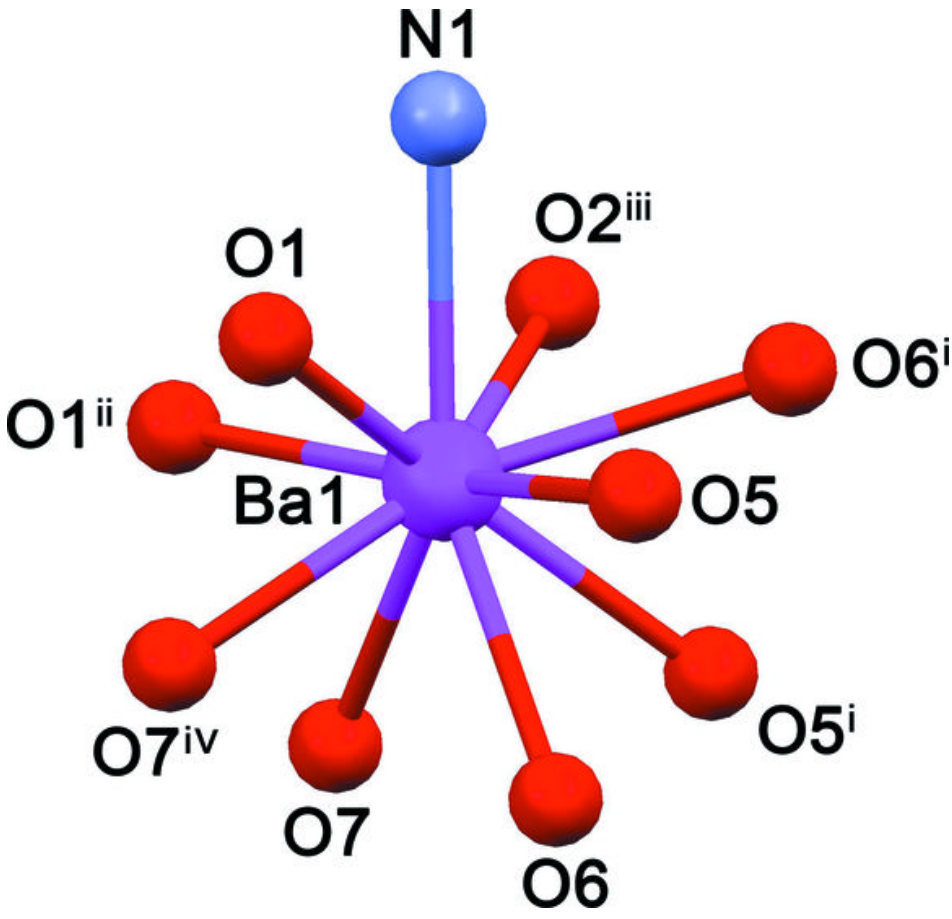


Fig. 3