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Poly[(μ_5-5-aminoisophthalato)aquabarium]

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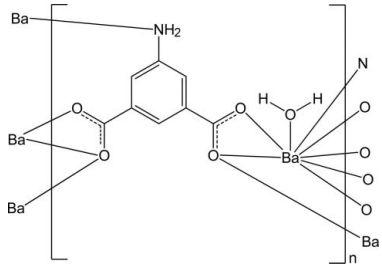
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.015; wR factor = 0.040; data-to-parameter ratio = 16.8.

In the title compound, $[Ba(C_8H_5NO_4)(H_2O)]_n$, the Ba^{II} ion is eight-coordinated by six O atoms and one N atom from five 5-aminoisophthalate ligands and one water molecule in a distorted dodecahedral geometry. The Ba^{II} ions are connected *via* the ligands into a layer parallel to (011). The layers are linked by N—H···O hydrogen bonds. The coordinated water molecule is involved in intralayer O—H···O hydrogen bonds.

Related literature

For general background to metal coordination polymers, see: Kitagawa *et al.* (2004). For related structures, see: Kongshaug & Fjellvåg (2006); Wu & Lin (2010); Zeng *et al.* (2007).



Experimental

Crystal data

$[Ba(C_8H_5NO_4)(H_2O)]$
M_r = 334.48
Triclinic, $P\overline{1}$
a = 7.7621 (1) Å
b = 7.9652 (1) Å
c = 8.3416 (1) Å
α = 79.618 (1)°
β = 65.574 (1)°
γ = 83.575 (1)°
V = 461.48 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.30 mm^{-1}
T = 295 K
0.50 × 0.30 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.232, T_{max} = 0.275
7950 measured reflections
2283 independent reflections
2230 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.040
S = 1.12
2283 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O3^{i}	0.89	1.90	2.770 (2)	165
O1W—H1WB···O2^{ii}	0.83	1.95	2.770 (2)	167
N1—H1A···O2^{iii}	0.96	2.16	3.067 (2)	157
N1—H1B···O4^{iv}	0.99	2.19	3.176 (2)	175

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2470).

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supplementary materials

Acta Cryst. (2011). E**67**, m1413 [**doi:10.1107/S1600536811037962**]

Poly[(μ_5-5-aminoisophthalato)aquabarium]

C.-Y. Wu and C.-H. Lin

Comment

The increasingly rapid development of metal coordination polymers over the past two decades has attracted considerable attention due to their structural diversity and important applications (Kitagawa *et al.*, 2004). 5-Aminoisophthalic acid has been successively reported as sodium (Zeng *et al.*, 2007), zinc (Kongshaug & Fjellvåg, 2006) and magnesium complexes (Wu & Lin, 2010). In our continuous investigations in metal coordination polymers, we report here the structure of a new Ba(II) coordination polymer based on the 5-aminoisophthalate ligand.

In the title compound (Fig. 1), the Ba^{II} ion is eight-coordinated by six O atoms and one N atom from five 5-aminoisophthalate ligands and one water molecule in a distorted dodecahedral geometry. The Ba—O distances range from 2.6808 (16) to 2.8813 (17) Å. The Ba—N distance is 2.918 (2) Å. The BaO_7N dodecahedra are connected *via* the anionic ligands into a layer parallel to (0 1 1). The coordinated water molecule is involved in intralayer O—H···O hydrogen bonds (Table 1 , Fig. 2). These layers are linked by interlayer N—H···O hydrogen bonds (Fig. 3).

Experimental

Solvothermal reactions were carried out at 423 K for 2 d in a Teflon-lined acid digestion bomb with an internal volume of 23 ml followed by slow cooling at 6 K h^{-1} to room temperature. A single-phase product consisting of transparent crystals was obtained from a mixture of 5-aminoisophthalic acid ($C_8H_7NO_4$, 0.145 g, 0.8 mmol), $Ba(NO_3)_2.4H_2O$ (0.105 g, 0.2 mmol), methanol (5.0 ml) and H_2O (1.0 ml).

Refinement

H atoms bound to C atoms were positioned geometrically, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms bound to N and O atoms were located in a difference Fourier map and fixed in refinements, with U_{iso}(H) = 1.5U_{eq}(O) or 1.2U_{eq}(N).

Figures

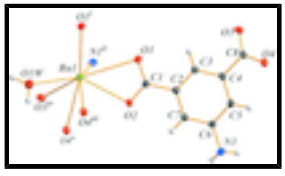

Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) -*x*, 1-*y*, 1-*z*; (ii) *x*, 1+*y*, *z*; (iii) -*x*, -*y*, 1-*z*; (iv) *x*, 1+*y*, -1+*z*.]

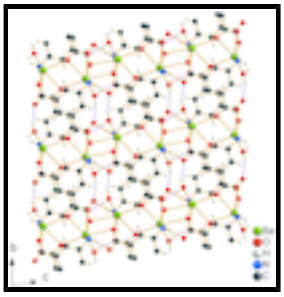

Fig. 2. The layer structure of the title compound viewed along the *a* axis. Intralayer O—H···O hydrogen bonds are shown as pink dashed lines.

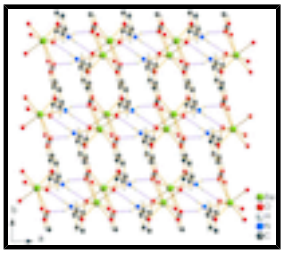

Fig. 3. The crystal packing of the title compound viewed along the *a* axis. Interlayer N—H···O hydrogen bonds are shown as pink dashed lines.

Poly[(μ$_5$-5-aminoisophthalato)aquabarium]

Crystal data

$[Ba(C_8H_5NO_4)(H_2O)]$	$Z = 2$
$M_r = 334.48$	$F(000) = 316$
Triclinic, $P\overline{1}$	$D_x = 2.407$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.7621$ (1) Å	Cell parameters from 120 reflections
$b = 7.9652$ (1) Å	$\theta = 2.6$–$31.8°$
$c = 8.3416$ (1) Å	$\mu = 4.30$ mm^{-1}
$\alpha = 79.618$ (1)°	$T = 295$ K
$\beta = 65.574$ (1)°	Block, colourless
$\gamma = 83.575$ (1)°	0.50 × 0.30 × 0.30 mm
$V = 461.48$ (1) Å^3	

Data collection

Bruker APEXII CCD diffractometer	2283 independent reflections
Radiation source: fine-focus sealed tube	2230 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.019$
Detector resolution: 8.3333 pixels mm^{-1}	$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$k = -10 \rightarrow 10$
$T_{min} = 0.232$, $T_{max} = 0.275$	$l = -11 \rightarrow 10$
7950 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.015$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.040$	H-atom parameters constrained
$S = 1.12$	$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2 + 0.2964P]$ where $P = (F_o^2 + 2F_c^2)/3$
2283 reflections	$(\Delta/\sigma)_{max} = 0.001$
136 parameters	$\Delta\rho_{max} = 0.48$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.79$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.047838 (16)	0.597922 (13)	0.212249 (13)	0.01817 (5)
O1	0.1383 (2)	0.32074 (19)	0.4588 (2)	0.0281 (3)
O1W	−0.1803 (3)	0.8279 (2)	0.0982 (2)	0.0345 (4)
H1WA	−0.1919	0.9411	0.0794	0.052*
H1WB	−0.2053	0.7847	0.0267	0.052*
O2	0.2226 (3)	0.27828 (19)	0.18144 (19)	0.0286 (3)
O3	0.2563 (3)	−0.1752 (2)	0.8942 (2)	0.0293 (3)
O4	0.2032 (2)	−0.42403 (18)	0.84296 (19)	0.0243 (3)
N1	0.4296 (3)	−0.3479 (2)	0.1704 (2)	0.0222 (3)
H1A	0.5246	−0.2931	0.0622	0.027*
H1B	0.5405	−0.4208	0.1747	0.027*
C1	0.2029 (3)	0.2256 (2)	0.3391 (3)	0.0198 (4)
C2	0.2556 (3)	0.0420 (2)	0.3867 (3)	0.0184 (4)
C3	0.2367 (3)	−0.0217 (2)	0.5594 (3)	0.0204 (4)
H3	0.1983	0.0512	0.6446	0.025*
C4	0.2751 (3)	−0.1940 (2)	0.6051 (3)	0.0180 (4)
C5	0.3385 (3)	−0.3012 (2)	0.4757 (3)	0.0191 (4)
H5	0.3610	−0.4171	0.5071	0.023*
C6	0.3688 (3)	−0.2373 (2)	0.2996 (3)	0.0179 (4)
C7	0.3232 (3)	−0.0654 (3)	0.2571 (3)	0.0193 (4)
H7	0.3382	−0.0221	0.1411	0.023*
C8	0.2440 (3)	−0.2676 (3)	0.7936 (3)	0.0191 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.02706 (8)	0.01489 (7)	0.01284 (7)	0.00289 (5)	−0.00903 (5)	−0.00259 (4)
O1	0.0457 (9)	0.0188 (7)	0.0174 (7)	0.0088 (6)	−0.0116 (7)	−0.0057 (6)
O1W	0.0527 (11)	0.0238 (8)	0.0411 (10)	0.0094 (7)	−0.0335 (9)	−0.0103 (7)
O2	0.0509 (10)	0.0182 (7)	0.0160 (7)	0.0084 (7)	−0.0156 (7)	−0.0020 (5)

O3	0.0511 (10)	0.0211 (7)	0.0205 (7)	−0.0045 (7)	−0.0190 (7)	−0.0013 (6)
O4	0.0381 (8)	0.0156 (7)	0.0187 (7)	−0.0021 (6)	−0.0125 (6)	0.0016 (5)
N1	0.0284 (9)	0.0191 (8)	0.0181 (8)	0.0046 (7)	−0.0081 (7)	−0.0065 (6)
C1	0.0266 (10)	0.0154 (9)	0.0153 (9)	0.0024 (7)	−0.0072 (8)	−0.0021 (7)
C2	0.0232 (9)	0.0162 (9)	0.0150 (9)	0.0025 (7)	−0.0078 (7)	−0.0018 (7)
C3	0.0298 (10)	0.0159 (9)	0.0145 (8)	0.0018 (7)	−0.0085 (8)	−0.0022 (7)
C4	0.0211 (9)	0.0177 (9)	0.0153 (8)	−0.0002 (7)	−0.0085 (7)	−0.0007 (7)
C5	0.0237 (9)	0.0145 (8)	0.0181 (9)	0.0023 (7)	−0.0090 (8)	−0.0005 (7)
C6	0.0193 (9)	0.0178 (9)	0.0165 (9)	0.0019 (7)	−0.0070 (7)	−0.0047 (7)
C7	0.0250 (9)	0.0173 (9)	0.0143 (8)	0.0022 (7)	−0.0078 (7)	−0.0012 (7)
C8	0.0244 (9)	0.0176 (9)	0.0149 (9)	0.0018 (7)	−0.0091 (7)	0.0001 (7)

Geometric parameters (Å, °)

Ba1—O1^{i}	2.6815 (15)	N1—C6	1.410 (2)
Ba1—O1W	2.7266 (16)	N1—H1A	0.9638
Ba1—O4^{ii}	2.7392 (16)	N1—H1B	0.9930
Ba1—O2	2.7502 (15)	C1—C2	1.502 (3)
Ba1—O4^{iii}	2.8371 (15)	C2—C3	1.390 (3)
Ba1—O3^{iii}	2.8807 (16)	C2—C7	1.393 (3)
Ba1—N1^{iv}	2.9094 (19)	C3—C4	1.390 (3)
Ba1—O1	2.9675 (15)	C3—H3	0.9300
O1—C1	1.263 (2)	C4—C5	1.391 (3)
O1W—H1WA	0.8880	C4—C8	1.504 (3)
O1W—H1WB	0.8346	C5—C6	1.394 (3)
O2—C1	1.256 (2)	C5—H5	0.9300
O3—C8	1.249 (2)	C6—C7	1.395 (3)
O4—C8	1.272 (2)	C7—H7	0.9300
O1^{i}—Ba1—O1W	89.50 (5)	O2—Ba1—Ba1^{v}	72.77 (3)
O1^{i}—Ba1—O4^{ii}	105.30 (5)	O4^{iii}—Ba1—Ba1^{v}	36.03 (3)
O1W—Ba1—O4^{ii}	71.13 (5)	O3^{iii}—Ba1—Ba1^{v}	76.62 (3)
O1^{i}—Ba1—O2	117.46 (4)	N1^{iv}—Ba1—Ba1^{v}	120.53 (3)
O1W—Ba1—O2	143.56 (5)	O1—Ba1—Ba1^{v}	112.75 (3)
O4^{ii}—Ba1—O2	77.97 (5)	C8^{iii}—Ba1—Ba1^{v}	54.33 (4)
O1^{i}—Ba1—O4^{iii}	167.63 (5)	C1—Ba1—Ba1^{v}	91.86 (4)
O1W—Ba1—O4^{iii}	78.43 (5)	C6^{iv}—Ba1—Ba1^{v}	143.55 (3)
O4^{ii}—Ba1—O4^{iii}	73.57 (5)	C1—O1—Ba1^{i}	157.18 (14)
O2—Ba1—O4^{iii}	74.63 (4)	C1—O1—Ba1	90.64 (12)
O1^{i}—Ba1—O3^{iii}	126.70 (5)	Ba1^{i}—O1—Ba1	106.97 (5)
O1W—Ba1—O3^{iii}	67.04 (5)	Ba1—O1W—H1WA	134.8
O4^{ii}—Ba1—O3^{iii}	110.30 (4)	Ba1—O1W—H1WB	107.5
O2—Ba1—O3^{iii}	107.93 (5)	H1WA—O1W—H1WB	111.2
O4^{iii}—Ba1—O3^{iii}	45.63 (4)	C1—O2—Ba1	101.23 (12)
O1^{i}—Ba1—N1^{iv}	97.88 (5)	C8—O3—Ba1^{vi}	93.35 (12)

O1W—Ba1—N1^{iv}	126.35 (5)	C8—O4—Ba1^{ii}	129.23 (13)
O4^{ii}—Ba1—N1^{iv}	151.39 (5)	C8—O4—Ba1^{vi}	94.88 (12)
O2—Ba1—N1^{iv}	76.55 (5)	Ba1^{ii}—O4—Ba1^{vi}	106.43 (5)
O4^{iii}—Ba1—N1^{iv}	87.26 (5)	C6—N1—Ba1^{vii}	94.09 (12)
O3^{iii}—Ba1—N1^{iv}	66.27 (5)	C6—N1—H1A	108.9
O1^{i}—Ba1—O1	73.03 (5)	Ba1^{vii}—N1—H1A	123.8
O1W—Ba1—O1	155.90 (5)	C6—N1—H1B	110.7
O4^{ii}—Ba1—O1	97.10 (4)	Ba1^{vii}—N1—H1B	136.5
O2—Ba1—O1	45.23 (4)	H1A—N1—H1B	82.2
O4^{iii}—Ba1—O1	119.31 (4)	O2—C1—O1	122.41 (18)
O3^{iii}—Ba1—O1	136.85 (5)	O2—C1—C2	118.51 (17)
N1^{iv}—Ba1—O1	73.66 (5)	O1—C1—C2	119.08 (17)
O1^{i}—Ba1—C8^{iii}	147.07 (5)	O2—C1—Ba1	56.41 (10)
O1W—Ba1—C8^{iii}	67.76 (5)	O1—C1—Ba1	66.40 (11)
O4^{ii}—Ba1—C8^{iii}	90.03 (5)	C2—C1—Ba1	170.98 (14)
O2—Ba1—C8^{iii}	93.92 (5)	C3—C2—C7	119.75 (18)
O4^{iii}—Ba1—C8^{iii}	23.28 (5)	C3—C2—C1	120.48 (17)
O3^{iii}—Ba1—C8^{iii}	22.89 (5)	C7—C2—C1	119.77 (17)
N1^{iv}—Ba1—C8^{iii}	78.98 (5)	C4—C3—C2	120.14 (18)
O1—Ba1—C8^{iii}	134.77 (5)	C4—C3—H3	119.9
O1^{i}—Ba1—C1	95.28 (5)	C2—C3—H3	119.9
O1W—Ba1—C1	156.97 (5)	C3—C4—C5	119.66 (17)
O4^{ii}—Ba1—C1	85.89 (5)	C3—C4—C8	121.00 (17)
O2—Ba1—C1	22.36 (4)	C5—C4—C8	119.32 (17)
O4^{iii}—Ba1—C1	96.91 (5)	C4—C5—C6	120.87 (17)
O3^{iii}—Ba1—C1	125.09 (5)	C4—C5—H5	119.6
N1^{iv}—Ba1—C1	75.35 (5)	C6—C5—H5	119.6
O1—Ba1—C1	22.96 (4)	C5—C6—C7	118.75 (17)
C8^{iii}—Ba1—C1	115.07 (5)	C5—C6—N1	120.32 (17)
O1^{i}—Ba1—C6^{iv}	74.74 (5)	C7—C6—N1	120.73 (18)
O1W—Ba1—C6^{iv}	115.84 (5)	C5—C6—Ba1^{vii}	107.12 (13)
O4^{ii}—Ba1—C6^{iv}	172.98 (5)	C7—C6—Ba1^{vii}	97.58 (12)
O2—Ba1—C6^{iv}	95.71 (5)	N1—C6—Ba1^{vii}	60.87 (10)
O4^{iii}—Ba1—C6^{iv}	107.94 (5)	C2—C7—C6	120.68 (18)
O3^{iii}—Ba1—C6^{iv}	74.39 (5)	C2—C7—H7	119.7
N1^{iv}—Ba1—C6^{iv}	25.04 (4)	C6—C7—H7	119.7
O1—Ba1—C6^{iv}	76.13 (5)	O3—C8—O4	123.16 (18)
C8^{iii}—Ba1—C6^{iv}	93.49 (5)	O3—C8—C4	119.92 (18)
C1—Ba1—C6^{iv}	87.11 (5)	O4—C8—C4	116.91 (17)
O1^{i}—Ba1—Ba1^{v}	141.47 (4)	O3—C8—Ba1^{vi}	63.76 (11)
O1W—Ba1—Ba1^{v}	70.99 (3)	O4—C8—Ba1^{vi}	61.84 (10)

O4^{ii}—Ba1—Ba1^{v}	37.54 (3)	C4—C8—Ba1^{vi}	162.79 (14)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O3^{i}	0.89	1.90	2.770 (2)	165
O1W—H1WB···O2^{v}	0.83	1.95	2.770 (2)	167
N1—H1A···O2^{viii}	0.96	2.16	3.067 (2)	157
N1—H1B···O4^{ix}	0.99	2.19	3.176 (2)	175

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (v) −*x*, −*y*+1, −*z*; (viii) −*x*+1, −*y*, −*z*; (ix) −*x*+1, −*y*−1, −*z*+1.

Fig. 1

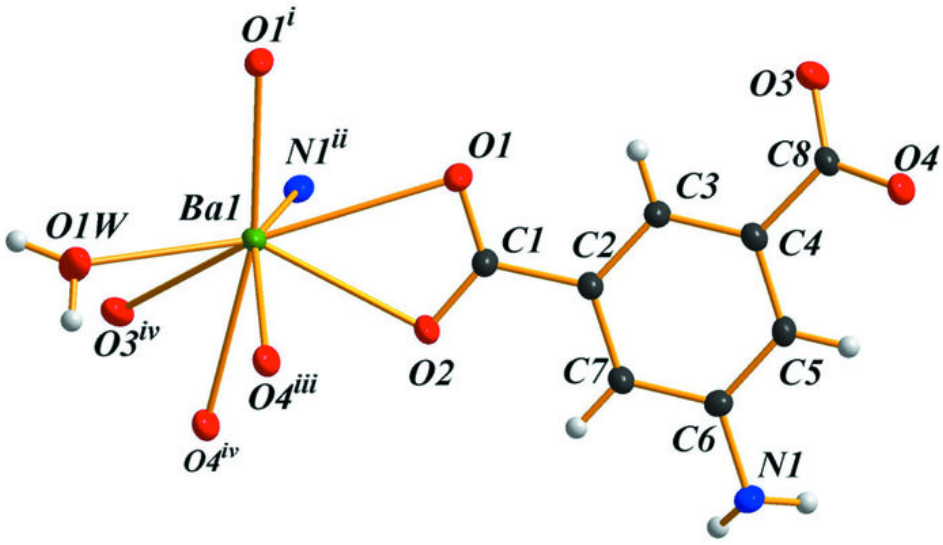
O1i
O3
N1ii
O1
C8
O4
C3
Ba1
O1W
C1
C2
C4
O3iv
O2
C7
C5
O4iii
C6
O4iv
N1

Fig. 2

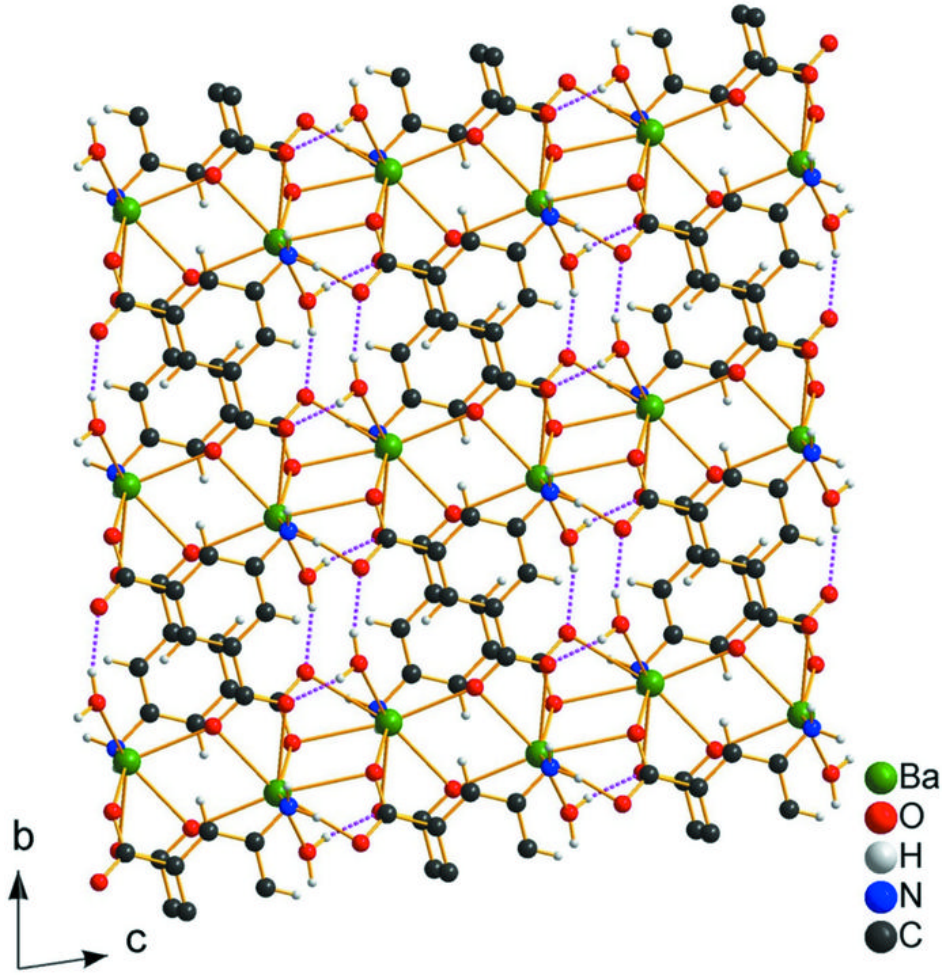

Fig. 3