

Poly[[diaqua(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato)strontium] monohydrate]

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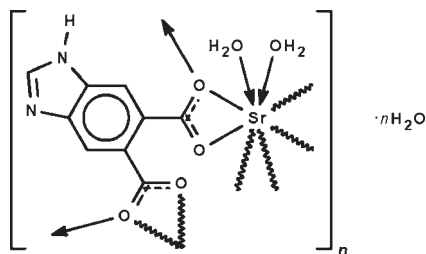
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.076; wR factor = 0.214; data-to-parameter ratio = 15.6.

Each of the carboxylate $-\text{CO}_2$ fragments of the dianion ligand in the title compound, $[\{\text{Sr}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2\}\cdot\text{H}_2\text{O}]_n$, chelates to a Sr^{II} atom and at the same time, one of the two O atoms coordinates to a third Sr^{II} atom. The μ_4 -bridging mode of the dianion generates a square-grid layer motif; adjacent layers are connected by $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a three-dimensional network. The eight-coordinate Sr atom exists in a distorted square-antiprismatic geometry. The crystal studied was a non-merohedral twin with a minor twin component of 24%.

Related literature

For the crystal structures of other metal salts of dicarboxylic acid, see: Gao *et al.* (2008); Lo *et al.* (2007); Song *et al.* (2009*a,b*). For the treated of diffraction data of twinned crystals, see: Spek (2009).



Experimental

Crystal data

$[\text{Sr}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}$ $b = 7.093$ (1) Å
 $M_r = 345.81$ $c = 13.037$ (2) Å
 Triclinic, $P\bar{1}$ $\alpha = 80.860$ (5)°
 $a = 6.909$ (1) Å $\beta = 83.974$ (5)°

$\gamma = 71.795$ (4)°
 $V = 598.2$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 4.54$ mm⁻¹
 $T = 293$ K
 $0.31 \times 0.24 \times 0.20$ mm

Data collection

Rigaku R-Axis RAPID IP diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.334$, $T_{\text{max}} = 0.464$

5799 measured reflections
 2695 independent reflections
 2339 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.076$
 $wR(F^2) = 0.214$
 $S = 1.05$
 2695 reflections

173 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 2.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -2.12$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sr1—O1	2.604 (5)	Sr1—O3 ⁱⁱⁱ	2.528 (5)
Sr1—O2	2.760 (5)	Sr1—O4 ⁱⁱ	2.635 (6)
Sr1—O2 ⁱ	2.516 (5)	Sr1—O1 _w	2.554 (5)
Sr1—O3 ⁱⁱ	2.711 (5)	Sr1—O2 _w	2.579 (6)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1 _w —H11 \cdots O1 ⁱⁱⁱ	0.84	1.98	2.81 (1)	167
O1 _w —H12 \cdots O4 ^{iv}	0.84	2.00	2.83 (1)	173
O2 _w —H21 \cdots O3 ^v	0.84	2.28	2.95 (1)	136
O2 _w —H22 \cdots O4 ⁱ	0.84	2.12	2.93 (1)	162
O3 _w —H3 _w 1 \cdots N1	0.84	1.97	2.78 (1)	160
O3 _w —H3 _w 2 \cdots O3 ^{vi}	0.84	2.39	3.01 (2)	132
N2—H2 _n \cdots O3 ^{vii}	0.88	2.07	2.75 (1)	134

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX* (Dolomanov *et al.*, 2003) and *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2672).

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supplementary materials

Acta Cryst. (2009). E65, m1643-m1644 [doi:10.1107/S1600536809048284]

Poly[[diaqua(μ_4 -1*H*-benzimidazole-5,6-dicarboxylato)strontium] monohydrate]

W.-D. Song, H. Wang, J.-H. Liu, X.-T. Ma and S. W. Ng

Experimental

Strontium dichloride hexahydrate (0.027 g, 0.1 mmol), 1*H*-benzimidazole-5,6-dicarboxylic acid (0.021 g, 0.1 mmol) and water (15 ml) along with a few drops of sodium hydroxide solution that adjusted the pH to about 7 were placed in a 25 ml glass vessel, which was kept at 277 K for several weeks. Colorless block-shaped crystals were obtained in 60% yield.

Refinement

Carbon- and nitrogen bound H-atoms were generated geometrically, and were constrained to ride on their parent atoms (C–H = 0.93 Å, $U = 1.5U_{\text{eq}}(\text{C})$; N–H 0.88 Å, $U = 1.2U_{\text{eq}}(\text{N})$).

For the two coordinated water molecules, their H-atoms rotated to fit the electron density. For the free water molecule, their H-atoms were placed in chemically sensible positions on the basis of hydrogen bonding interactions; O–H = 0.84 Å. Their temperature factors were similarly tied. The short intermolecular H3w2...H3w2 contact of < 2.0 Å may be an artifact of possible disorder in the O3w water molecule. However, it was not necessary, to split it into two components.

The structure is a non-merohedral twin; the diffraction intensities were split into two components by *PLATON* (Spek, 2009).

The final difference Fourier map had a large peak/deep hole in the vicinity of Sr1.

Figures

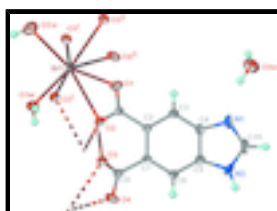


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a portion of the chain structure of $\text{Sr}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_4\text{N}_2\text{O}_2)\cdot\text{H}_2\text{O}$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

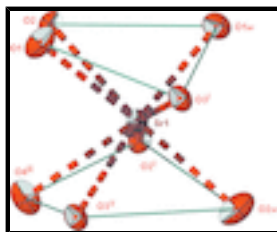


Fig. 2. Detail of the geometry of Sr1.

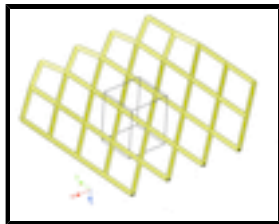


Fig. 3. OLEX (Dolomanov *et al.*, 2003) depiction of the layer motif.

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Crystal data

[Sr(C ₉ H ₄ N ₂ O ₄)(H ₂ O) ₂] \cdot H ₂ O	$Z = 2$
$M_r = 345.81$	$F_{000} = 344$
Triclinic, PT	$D_x = 1.920 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.909 (1) \text{ \AA}$	Cell parameters from 5129 reflections
$b = 7.093 (1) \text{ \AA}$	$\theta = 3.1\text{--}27.5^\circ$
$c = 13.037 (2) \text{ \AA}$	$\mu = 4.54 \text{ mm}^{-1}$
$\alpha = 80.860 (5)^\circ$	$T = 293 \text{ K}$
$\beta = 83.974 (5)^\circ$	Block, colorless
$\gamma = 71.795 (4)^\circ$	$0.31 \times 0.24 \times 0.20 \text{ mm}$
$V = 598.2 (2) \text{ \AA}^3$	

Data collection

Rigaku R-Axis RAPID IP diffractometer	2695 independent reflections
Radiation source: fine-focus sealed tube	2339 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.075$
$T = 293 \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scan	$\theta_{\text{min}} = 3.1^\circ$
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.334$, $T_{\text{max}} = 0.464$	$k = -9 \rightarrow 9$
5799 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.076$	H-atom parameters constrained
$wR(F^2) = 0.214$	$w = 1/[\sigma^2(F_o^2) + (0.1352P)^2 + 1.3937P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
2695 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
	$\Delta\rho_{\text{max}} = 2.69 \text{ e \AA}^{-3}$

173 parameters

$$\Delta\rho_{\min} = -2.12 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.25457 (8)	0.25734 (8)	0.46107 (4)	0.0207 (3)
O1	0.4011 (8)	0.3453 (8)	0.6171 (5)	0.0353 (13)
O2	0.1154 (7)	0.5758 (7)	0.5744 (4)	0.0261 (10)
O3	0.3642 (7)	0.8869 (7)	0.5721 (4)	0.0268 (10)
O4	0.0729 (8)	1.0928 (8)	0.6225 (5)	0.0401 (14)
O1w	0.2542 (8)	0.5682 (8)	0.3316 (4)	0.0327 (12)
H11	0.3596	0.6002	0.3370	0.049*
H12	0.1502	0.6631	0.3443	0.049*
O2w	0.2942 (10)	0.0310 (10)	0.3189 (6)	0.0502 (17)
H21	0.3087	0.0953	0.2602	0.075*
H22	0.1896	-0.0064	0.3213	0.075*
O3w	0.3469 (12)	0.0350 (11)	1.0913 (6)	0.0594 (19)
H3w1	0.3165	0.1485	1.0555	0.089*
H3w2	0.4687	-0.0248	1.0740	0.089*
N1	0.2543 (11)	0.4413 (11)	1.0195 (5)	0.0378 (16)
N2	0.1892 (12)	0.7679 (11)	1.0241 (5)	0.0387 (16)
H2N	0.1640	0.8830	1.0480	0.046*
C1	0.2549 (10)	0.4986 (9)	0.6338 (5)	0.0198 (12)
C2	0.2500 (9)	0.5836 (9)	0.7336 (5)	0.0192 (12)
C3	0.2665 (11)	0.4524 (10)	0.8249 (6)	0.0254 (14)
H3	0.2916	0.3160	0.8239	0.031*
C4	0.2448 (11)	0.5298 (11)	0.9184 (6)	0.0281 (15)
C5	0.2019 (11)	0.7366 (11)	0.9214 (6)	0.0276 (14)
C6	0.1836 (11)	0.8687 (10)	0.8295 (6)	0.0267 (14)
H6	0.1550	1.0055	0.8308	0.032*
C7	0.2086 (9)	0.7926 (9)	0.7361 (5)	0.0190 (12)
C8	0.2165 (9)	0.9307 (9)	0.6363 (5)	0.0216 (13)
C10	0.2225 (14)	0.5909 (14)	1.0781 (6)	0.042 (2)
H10	0.2243	0.5692	1.1503	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0175 (4)	0.0190 (4)	0.0219 (4)	-0.0002 (2)	-0.0012 (2)	-0.0025 (3)
O1	0.027 (3)	0.032 (3)	0.042 (3)	0.008 (2)	-0.010 (2)	-0.017 (2)
O2	0.022 (2)	0.028 (2)	0.026 (3)	-0.0030 (18)	-0.0043 (19)	-0.007 (2)
O3	0.020 (2)	0.026 (2)	0.029 (3)	-0.0029 (18)	0.0065 (19)	-0.002 (2)
O4	0.030 (3)	0.026 (3)	0.045 (3)	0.011 (2)	0.010 (2)	0.005 (2)
O1w	0.026 (3)	0.030 (3)	0.039 (3)	-0.006 (2)	0.004 (2)	-0.004 (2)
O2w	0.047 (4)	0.051 (4)	0.057 (4)	-0.009 (3)	-0.012 (3)	-0.024 (3)
O3w	0.066 (5)	0.045 (4)	0.066 (5)	-0.016 (3)	-0.013 (4)	0.001 (4)

supplementary materials

N1	0.049 (4)	0.045 (4)	0.020 (3)	-0.018 (3)	-0.005 (3)	0.000 (3)
N2	0.055 (4)	0.039 (4)	0.024 (3)	-0.011 (3)	0.000 (3)	-0.017 (3)
C1	0.018 (3)	0.020 (3)	0.022 (3)	-0.004 (2)	0.000 (2)	-0.005 (2)
C2	0.014 (3)	0.019 (3)	0.022 (3)	-0.001 (2)	-0.002 (2)	-0.005 (2)
C3	0.032 (4)	0.020 (3)	0.027 (4)	-0.009 (2)	-0.002 (3)	-0.005 (3)
C4	0.035 (4)	0.030 (4)	0.021 (4)	-0.012 (3)	-0.005 (3)	-0.001 (3)
C5	0.033 (4)	0.027 (3)	0.025 (4)	-0.011 (3)	-0.003 (3)	-0.005 (3)
C6	0.034 (4)	0.019 (3)	0.026 (4)	-0.007 (3)	0.000 (3)	-0.004 (3)
C7	0.020 (3)	0.015 (3)	0.021 (3)	-0.004 (2)	0.002 (2)	-0.003 (2)
C8	0.016 (3)	0.021 (3)	0.025 (3)	0.000 (2)	-0.001 (2)	-0.008 (3)
C10	0.049 (5)	0.058 (5)	0.018 (4)	-0.013 (4)	-0.006 (3)	0.000 (3)

Geometric parameters (Å, °)

Sr1—O1	2.604 (5)	O2w—H22	0.8400
Sr1—O2	2.760 (5)	O3w—H3w1	0.8400
Sr1—O2 ⁱ	2.516 (5)	O3w—H3w2	0.8400
Sr1—O3 ⁱⁱ	2.711 (5)	N1—C10	1.354 (11)
Sr1—O3 ⁱⁱⁱ	2.528 (5)	N1—C4	1.366 (9)
Sr1—O4 ⁱⁱ	2.635 (6)	N2—C10	1.302 (11)
Sr1—O1w	2.554 (5)	N2—C5	1.381 (9)
Sr1—O2w	2.579 (6)	N2—H2N	0.8800
O1—C1	1.262 (8)	C1—C2	1.511 (9)
O2—C1	1.233 (8)	C2—C3	1.382 (10)
O2—Sr1 ⁱ	2.516 (5)	C2—C7	1.424 (8)
O3—C8	1.242 (8)	C3—C4	1.390 (10)
O3—Sr1 ⁱⁱⁱ	2.528 (5)	C3—H3	0.9300
O3—Sr1 ^{iv}	2.711 (5)	C4—C5	1.409 (9)
O4—C8	1.264 (8)	C5—C6	1.390 (10)
O4—Sr1 ^{iv}	2.635 (6)	C6—C7	1.383 (9)
O1w—H11	0.8400	C6—H6	0.9300
O1w—H12	0.8400	C7—C8	1.506 (9)
O2w—H21	0.8400	C10—H10	0.9300
O2 ⁱ —Sr1—O3 ⁱⁱⁱ	159.81 (17)	Sr1—O1w—H12	109.5
O2 ⁱ —Sr1—O1w	75.51 (17)	H11—O1w—H12	109.5
O3 ⁱⁱⁱ —Sr1—O1w	90.53 (16)	Sr1—O2w—H21	109.5
O2 ⁱ —Sr1—O2w	90.93 (18)	Sr1—O2w—H22	109.5
O3 ⁱⁱⁱ —Sr1—O2w	75.39 (19)	H21—O2w—H22	109.5
O1w—Sr1—O2w	94.2 (2)	H3w1—O3w—H3w2	107.1
O2 ⁱ —Sr1—O1	118.96 (15)	C10—N1—C4	106.1 (7)
O3 ⁱⁱⁱ —Sr1—O1	77.00 (17)	C10—N2—C5	105.4 (7)
O1w—Sr1—O1	98.63 (19)	C10—N2—H2N	127.3
O2w—Sr1—O1	149.54 (18)	C5—N2—H2N	127.3
O2 ⁱ —Sr1—O4 ⁱⁱ	78.71 (17)	O2—C1—O1	122.9 (6)
O3 ⁱⁱⁱ —Sr1—O4 ⁱⁱ	118.75 (16)	O2—C1—C2	119.6 (6)

O1w—Sr1—O4 ⁱⁱ	148.09 (16)	O1—C1—C2	117.4 (6)
O2w—Sr1—O4 ⁱⁱ	104.7 (2)	C3—C2—C7	120.5 (6)
O1—Sr1—O4 ⁱⁱ	77.8 (2)	C3—C2—C1	117.0 (5)
O2 ⁱ —Sr1—O3 ⁱⁱ	118.90 (16)	C7—C2—C1	122.2 (6)
O3 ⁱⁱⁱ —Sr1—O3 ⁱⁱ	73.35 (17)	C2—C3—C4	118.1 (6)
O1w—Sr1—O3 ⁱⁱ	163.41 (16)	C2—C3—H3	120.9
O2w—Sr1—O3 ⁱⁱ	78.2 (2)	C4—C3—H3	120.9
O1—Sr1—O3 ⁱⁱ	81.86 (17)	N1—C4—C3	132.1 (7)
O4 ⁱⁱ —Sr1—O3 ⁱⁱ	48.37 (14)	N1—C4—C5	106.2 (6)
O2 ⁱ —Sr1—O2	72.84 (17)	C3—C4—C5	121.7 (7)
O3 ⁱⁱⁱ —Sr1—O2	117.87 (16)	N2—C5—C6	131.4 (7)
O1w—Sr1—O2	74.33 (16)	N2—C5—C4	108.4 (6)
O2w—Sr1—O2	161.91 (19)	C6—C5—C4	120.1 (7)
O1—Sr1—O2	48.13 (14)	C7—C6—C5	118.6 (6)
O4 ⁱⁱ —Sr1—O2	80.35 (17)	C7—C6—H6	120.7
O3 ⁱⁱ —Sr1—O2	116.38 (15)	C5—C6—H6	120.7
O1—Sr1—C8 ⁱⁱ	76.73 (18)	C6—C7—C2	121.0 (6)
C1—O1—Sr1	97.5 (4)	C6—C7—C8	118.7 (5)
C1—O2—Sr1 ⁱ	152.2 (5)	C2—C7—C8	119.9 (6)
C1—O2—Sr1	90.8 (4)	O3—C8—O4	122.0 (7)
Sr1 ⁱ —O2—Sr1	107.16 (17)	O3—C8—C7	120.0 (5)
C8—O3—Sr1 ⁱⁱⁱ	148.1 (5)	O4—C8—C7	117.9 (6)
C8—O3—Sr1 ^{iv}	92.8 (4)	N2—C10—N1	113.9 (7)
Sr1 ⁱⁱⁱ —O3—Sr1 ^{iv}	106.65 (17)	N2—C10—H10	123.0
C8—O4—Sr1 ^{iv}	95.9 (4)	N1—C10—H10	123.0
Sr1—O1w—H11	109.5		
O2 ⁱ —Sr1—O1—C1	-13.7 (5)	C1—C2—C3—C4	-174.6 (6)
O3 ⁱⁱⁱ —Sr1—O1—C1	153.0 (5)	C10—N1—C4—C3	179.6 (8)
O1w—Sr1—O1—C1	64.5 (5)	C10—N1—C4—C5	-1.3 (9)
O2w—Sr1—O1—C1	178.4 (4)	C2—C3—C4—N1	-179.4 (8)
O4 ⁱⁱ —Sr1—O1—C1	-83.2 (4)	C2—C3—C4—C5	1.6 (10)
O3 ⁱⁱ —Sr1—O1—C1	-132.3 (5)	C10—N2—C5—C6	-178.7 (9)
O2—Sr1—O1—C1	4.7 (4)	C10—N2—C5—C4	0.0 (9)
O2 ⁱ —Sr1—O2—C1	158.5 (5)	N1—C4—C5—N2	0.8 (9)
O3 ⁱⁱⁱ —Sr1—O2—C1	-40.1 (4)	C3—C4—C5—N2	-180.0 (7)
O1w—Sr1—O2—C1	-122.2 (4)	N1—C4—C5—C6	179.7 (7)
O2w—Sr1—O2—C1	-174.5 (6)	C3—C4—C5—C6	-1.1 (11)
O1—Sr1—O2—C1	-4.8 (4)	N2—C5—C6—C7	178.5 (8)
O4 ⁱⁱ —Sr1—O2—C1	77.4 (4)	C4—C5—C6—C7	-0.1 (11)
O3 ⁱⁱ —Sr1—O2—C1	44.2 (4)	C5—C6—C7—C2	0.7 (10)
O2 ⁱ —Sr1—O2—Sr1 ⁱ	0.0	C5—C6—C7—C8	-172.0 (6)
O3 ⁱⁱⁱ —Sr1—O2—Sr1 ⁱ	161.42 (17)	C3—C2—C7—C6	-0.2 (9)

supplementary materials

O1w—Sr1—O2—Sr1 ⁱ	79.3 (2)	C1—C2—C7—C6	173.1 (6)
O2w—Sr1—O2—Sr1 ⁱ	27.0 (7)	C3—C2—C7—C8	172.4 (6)
O1—Sr1—O2—Sr1 ⁱ	-163.2 (3)	C1—C2—C7—C8	-14.3 (9)
O4 ⁱⁱ —Sr1—O2—Sr1 ⁱ	-81.1 (2)	Sr1 ⁱⁱⁱ —O3—C8—O4	138.1 (7)
O3 ⁱⁱ —Sr1—O2—Sr1 ⁱ	-114.29 (18)	Sr1 ^{iv} —O3—C8—O4	9.6 (7)
Sr1 ⁱ —O2—C1—O1	139.9 (8)	Sr1 ⁱⁱⁱ —O3—C8—C7	-39.6 (12)
Sr1—O2—C1—O1	8.8 (7)	Sr1 ^{iv} —O3—C8—C7	-168.1 (5)
Sr1 ⁱ —O2—C1—C2	-37.6 (12)	Sr1 ^{iv} —O4—C8—O3	-9.9 (7)
Sr1—O2—C1—C2	-168.8 (5)	Sr1 ^{iv} —O4—C8—C7	167.8 (5)
Sr1—O1—C1—O2	-9.4 (8)	C6—C7—C8—O3	125.0 (7)
Sr1—O1—C1—C2	168.3 (5)	C2—C7—C8—O3	-47.8 (9)
O2—C1—C2—C3	125.8 (7)	C6—C7—C8—O4	-52.8 (9)
O1—C1—C2—C3	-51.9 (9)	C2—C7—C8—O4	134.4 (7)
O2—C1—C2—C7	-47.7 (9)	C5—N2—C10—N1	-0.9 (10)
O1—C1—C2—C7	134.6 (7)	C4—N1—C10—N2	1.4 (10)
C7—C2—C3—C4	-0.9 (9)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1w—H11...O1 ⁱⁱⁱ	0.84	1.98	2.81 (1)	167
O1w—H12...O4 ^v	0.84	2.00	2.83 (1)	173
O2w—H21...O3w ^{vi}	0.84	2.28	2.95 (1)	136
O2w—H22...O4 ⁱ	0.84	2.12	2.93 (1)	162
O3w—H3w1...N1	0.84	1.97	2.78 (1)	160
O3w—H3w2...O3w ^{vii}	0.84	2.39	3.01 (2)	132
N2—H2n...O3w ^{iv}	0.88	2.07	2.75 (1)	134

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

Fig. 1

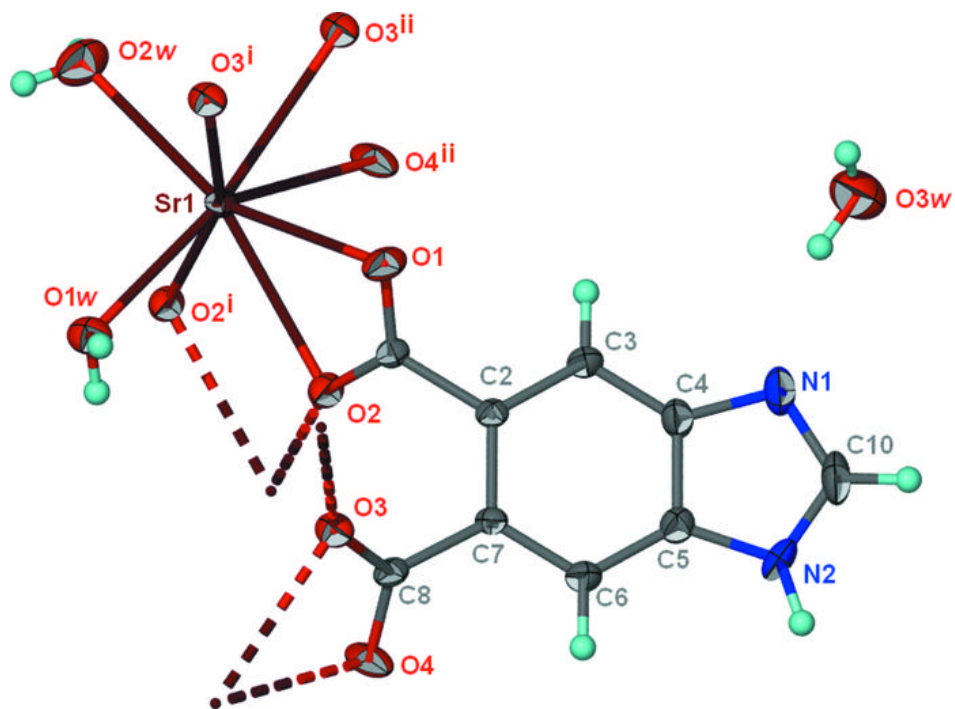


Fig. 2

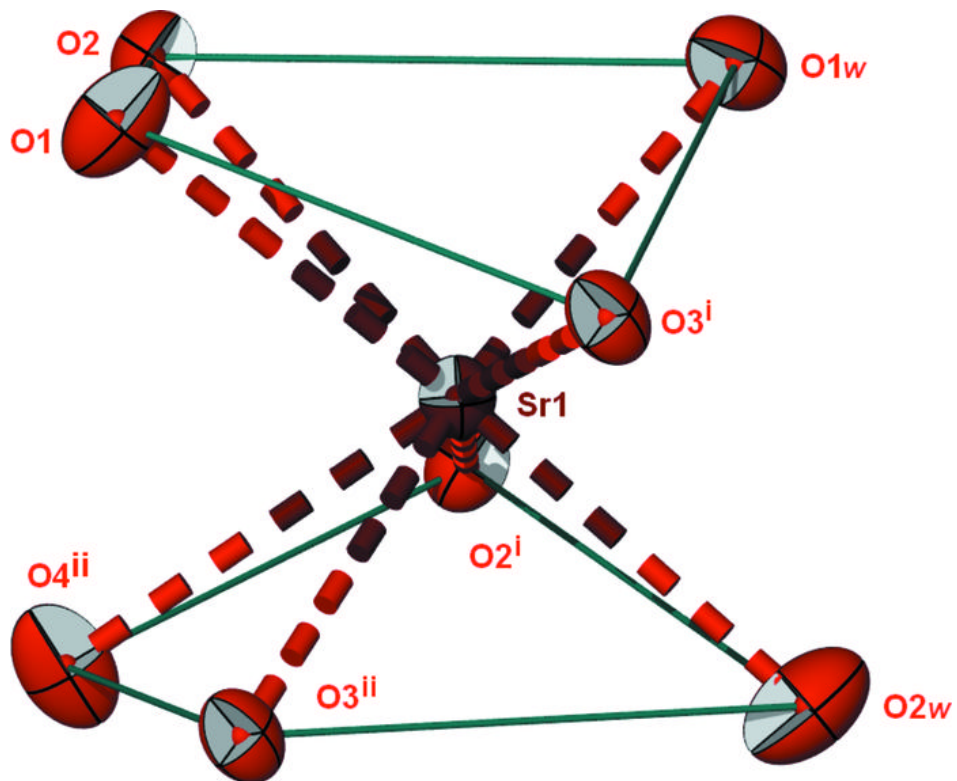


Fig. 3

