

Poly[[diaqua- μ_4 -pyrazine-2,3-dicarboxylato- $\kappa^6N,O^2:O^2':O^3,O^3':O^3$ -strontium(II)] monohydrate]

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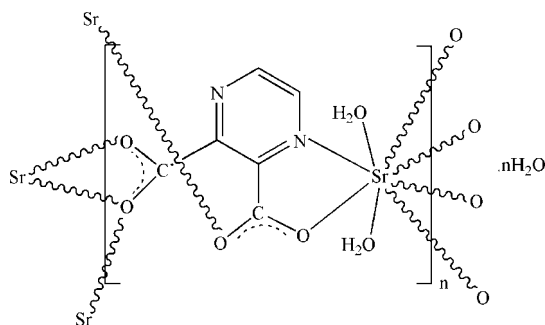
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.025; wR factor = 0.055; data-to-parameter ratio = 13.3.

In the title compound, $\{[Sr(C_6H_2N_2O_4)(H_2O)_2] \cdot H_2O\}_n$, the Sr^{II} ions are bridged by the pyrazine-2,3-dicarboxylate ligands with the formation of two-dimensional polymeric layers parallel to the ac plane. Each Sr^{II} ion is eight-coordinated by one N and five O atoms from the four ligands and two water molecules. The coordination polyhedron is derived from a pentagonal bipyramid with an O atom at the apex on one side of the equatorial plane and two O atoms sharing the apical site on the other side. The coordinated and uncoordinated water molecules are involved in $O-H \cdots O$ and $O-H \cdots N$ hydrogen bonds, which consolidate the crystal structure.

Related literature

For related literature, see: Takusagawa & Shimada (1973); Richard *et al.* (1973); Zou *et al.* (1999); Konar *et al.* (2004); Li *et al.* (2003); Xu *et al.* (2008); Ma *et al.* (2006); Ptasiewicz-Bak & Leciejewicz (1997*a,b*); Starosta & Leciejewicz (2005); Tombul *et al.* (2006).



Experimental

Crystal data

$[Sr(C_6H_2N_2O_4)(H_2O)_2] \cdot H_2O$
 $M_r = 307.76$
 Monoclinic, $P2_1/n$
 $a = 10.4931$ (7) Å
 $b = 6.9839$ (4) Å
 $c = 13.5208$ (8) Å
 $\beta = 94.2670$ (10)°

$V = 988.10$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.48$ mm⁻¹
 $T = 120$ (2) K
 $0.28 \times 0.25 \times 0.10$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{min} = 0.240$, $T_{max} = 0.568$

8338 measured reflections
 1934 independent reflections
 1595 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.054$
 $S = 1.00$
 1934 reflections

145 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.92$ e Å⁻³
 $\Delta\rho_{min} = -0.45$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sr1—O2 ⁱ	2.4887 (18)	Sr1—O3	2.6145 (18)
Sr1—O2W	2.5106 (18)	Sr1—O1 ⁱⁱⁱ	2.6155 (18)
Sr1—O4 ⁱⁱ	2.5533 (18)	Sr1—N1	2.714 (2)
Sr1—O1W	2.5937 (19)	Sr1—O2 ⁱⁱⁱ	2.8517 (18)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1W1 \cdots O3W ⁱ	0.85	1.87	2.713 (3)	170
O1W—H2W1 \cdots O3W ^{iv}	0.85	1.90	2.744 (3)	171
O2W—H1W2 \cdots O1 ⁱⁱ	0.85	1.85	2.696 (3)	174
O2W—H2W2 \cdots O1W ^v	0.85	2.01	2.857 (3)	178
O3W—H1W3 \cdots O4	0.85	1.94	2.781 (3)	170
O3W—H2W3 \cdots N2 ^{vi}	0.85	1.96	2.792 (3)	168

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1998); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; 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: CV2408).

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supplementary materials

Acta Cryst. (2008). E64, m888-m889 [doi:10.1107/S1600536808015316]

Poly[[diaqua- μ_4 -pyrazine-2,3-dicarboxylato- $\kappa^6 N, O^2:O^2':O^3, O^3':O^3$ -strontium(II)] monohydrate]

A. Abedi, M. Mousavi Mirkolaei and V. Amani

Comment

Takusagawa & Shimada (1973) first determined the structure of pyrazine-2,3-dicarboxylic acid by single-crystal X-ray analysis. Almost at the same time, the first metal-organic compound of pyrazine-2,3-dicarboxylic acid was reported (Richard *et al.*, 1973). Among many reported compounds containing pyrazine-2,3-dicarboxylic acid, most are complexes of transition metal ions, including manganese (Zou *et al.*, 1999), copper (Konar *et al.*, 2004), zinc (Li *et al.*, 2003), iron (Xu *et al.*, 2008) and cadmium (Ma *et al.*, 2006). Also, there are many reported compounds of pyrazine-2,3-dicarboxylic acid with main group metals such as calcium (Ptasiewicz-Bak & Leciejewicz, 1997*a*; Starosta & Leciejewicz, 2005), magnesium (Ptasiewicz-Bak & Leciejewicz, 1997*b*) and sodium (Tombul *et al.*, 2006) complexes. For further investigation of pyrazine-2,3-dicarboxylic acid, we synthesized the title compound, (I).

The asymmetric unit of the title compound, (Fig. 1), contains molecular sheets in which Sr^{II} ions are bridged by the carboxylate groups of the ligand molecules. Two bridging paths are evident. In the first, an N,O-bonding moiety formed by a hetero-ring nitrogen atom and the carboxylate oxygen atom nearest to it and both oxygen atoms of the second carboxylic group are active. The second path is formed by the other oxygen atom from the carboxylic group involved in the N,O-bonding moiety and an oxygen atom from the second carboxylic group. The latter atom is bidentate. A two-dimensional molecular pattern is formed. Each Sr^{II} ion is also coordinated by two water oxygen atoms, making the number of coordinated atoms eight. The coordination polyhedron is a distorted pentagonal bipyramid with an oxygen atom at the apex on one side of the equatorial plane and two oxygen atoms forming the apices on the other side. There is also one non-coordinated water molecule in the asymmetric unit. The Sr—O and Sr—N bond lengths are collected in Table 1.

Intermolecular O—H \cdots O and O—H \cdots N hydrogen bonds (Table 2) help to consolidate the crystal packing (Fig. 2).

Experimental

A solution of pyrazine-2,3-dicarboxylic acid (0.5 g, 2.91 mmol) in methanol (40 ml) was added to a solution of Sr(NO₃)₂ (0.31 g, 1.46 mmol) in water (10 ml) and the resulting colourless solution was stirred for 10 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colourless plate crystals of the title compound were isolated (yield 0.35 g, 78.03%).

Refinement

C-bound H atoms were geometrically positioned (C—H 0.95 Å), while O-bound H atoms were found in difference Fourier maps, but placed in idealized positions with O—H of 0.85 Å. All hydrogen atoms were refined in riding model approximation with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the parent atom.

Figures

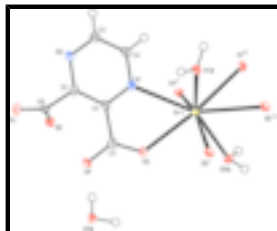


Fig. 1. A portion of the polymeric structure of (I) with the atom-numbering scheme and displacement ellipsoids drawn at the 40% probability level [symmetry codes: (i) $-x - 1/2, y - 1/2, -z + 1/2$, (ii) $-x - 1/2, y + 1/2, -z + 1/2$, (iii) $x - 1/2, -y + 1/2, z + 1/2$].

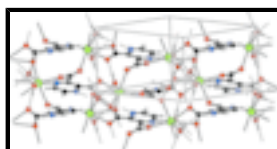


Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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Crystal data

$[\text{Sr}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$

$M_r = 307.76$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 10.4931\ (7)\ \text{\AA}$

$b = 6.9839\ (4)\ \text{\AA}$

$c = 13.5208\ (8)\ \text{\AA}$

$\beta = 94.2670\ (10)^\circ$

$V = 988.10\ (10)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 608$

$D_x = 2.069\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 156 reflections

$\theta = 3\text{--}26^\circ$

$\mu = 5.48\ \text{mm}^{-1}$

$T = 120\ (2)\ \text{K}$

Plate, colorless

$0.28 \times 0.25 \times 0.10\ \text{mm}$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 120(2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 1998)

$T_{\min} = 0.240, T_{\max} = 0.568$

8338 measured reflections

1934 independent reflections

1595 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.4^\circ$

$h = -12 \rightarrow 12$

$k = -8 \rightarrow 8$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

$$R[F^2 > 2\sigma(F^2)] = 0.024$$

$$wR(F^2) = 0.054$$

$$S = 1.01$$

1934 reflections

145 parameters

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.026P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.92 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	-0.44206 (2)	0.17756 (3)	0.375530 (17)	0.01058 (9)
N1	-0.4291 (2)	0.1488 (3)	0.17632 (16)	0.0137 (5)
N2	-0.3958 (2)	0.2550 (3)	-0.01781 (16)	0.0138 (5)
O1	-0.14140 (18)	0.1344 (3)	-0.07125 (13)	0.0154 (4)
O2	-0.09707 (18)	0.3655 (3)	0.03862 (13)	0.0148 (4)
O3	-0.21964 (18)	0.1162 (3)	0.30617 (13)	0.0164 (4)
O4	-0.10633 (16)	0.0171 (3)	0.18088 (13)	0.0131 (4)
C1	-0.3115 (2)	0.1518 (4)	0.14221 (19)	0.0114 (6)
C2	-0.2956 (3)	0.2059 (4)	0.04464 (19)	0.0117 (6)
C3	-0.5114 (3)	0.2480 (4)	0.0166 (2)	0.0156 (6)
H3A	-0.5841	0.2794	-0.0264	0.019*
C4	-0.5277 (3)	0.1963 (4)	0.11335 (19)	0.0150 (6)
H4A	-0.6115	0.1945	0.1356	0.018*
C5	-0.2037 (3)	0.0901 (4)	0.21630 (19)	0.0123 (6)
C6	-0.1670 (3)	0.2340 (4)	0.00239 (19)	0.0114 (6)
O1W	-0.64324 (17)	-0.0101 (3)	0.30768 (13)	0.0161 (4)
H1W1	-0.6382	-0.1106	0.2727	0.019*
H2W1	-0.7174	0.0355	0.2932	0.019*
O2W	-0.31193 (17)	0.2633 (3)	0.53262 (13)	0.0150 (4)
H1W2	-0.3220	0.3802	0.5478	0.018*
H2W2	-0.3246	0.1853	0.5791	0.018*
O3W	0.11689 (17)	0.1471 (3)	0.28299 (13)	0.0161 (4)
H1W3	0.0444	0.1203	0.2540	0.019*
H2W3	0.1011	0.1787	0.3415	0.019*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00953 (13)	0.01224 (14)	0.01019 (13)	0.00004 (11)	0.00220 (9)	0.00048 (11)
N1	0.0110 (12)	0.0183 (13)	0.0119 (11)	0.0000 (10)	0.0026 (9)	-0.0003 (10)
N2	0.0112 (12)	0.0163 (12)	0.0140 (11)	0.0013 (9)	0.0021 (9)	0.0000 (10)
O1	0.0168 (10)	0.0174 (10)	0.0125 (9)	-0.0015 (8)	0.0050 (8)	-0.0024 (8)
O2	0.0123 (10)	0.0160 (11)	0.0163 (10)	-0.0026 (8)	0.0029 (8)	-0.0017 (8)
O3	0.0142 (10)	0.0245 (11)	0.0106 (9)	0.0028 (8)	0.0022 (8)	-0.0006 (8)
O4	0.0084 (9)	0.0159 (10)	0.0154 (9)	0.0020 (8)	0.0033 (8)	-0.0022 (8)
C1	0.0086 (13)	0.0133 (14)	0.0124 (13)	-0.0008 (11)	0.0016 (10)	-0.0041 (11)
C2	0.0137 (14)	0.0095 (13)	0.0123 (13)	-0.0030 (11)	0.0024 (11)	-0.0016 (11)
C3	0.0119 (15)	0.0185 (14)	0.0161 (14)	0.0013 (11)	-0.0009 (11)	-0.0008 (12)
C4	0.0096 (14)	0.0195 (15)	0.0157 (14)	-0.0006 (11)	0.0005 (11)	-0.0008 (12)
C5	0.0126 (14)	0.0099 (13)	0.0144 (14)	-0.0027 (11)	0.0017 (11)	0.0027 (11)
C6	0.0115 (14)	0.0108 (13)	0.0118 (13)	0.0017 (11)	-0.0001 (11)	0.0027 (11)
O1W	0.0123 (10)	0.0176 (10)	0.0184 (10)	0.0009 (8)	0.0016 (8)	-0.0007 (8)
O2W	0.0161 (10)	0.0145 (10)	0.0142 (10)	-0.0007 (8)	0.0010 (8)	0.0013 (8)
O3W	0.0112 (10)	0.0257 (11)	0.0113 (9)	-0.0009 (8)	0.0012 (8)	-0.0013 (8)

Geometric parameters (\AA , $^\circ$)

Sr1—O2 ⁱ	2.4887 (18)	O2—Sr1 ⁱⁱ	2.4887 (18)
Sr1—O2W	2.5106 (18)	O2—Sr1 ^v	2.8517 (18)
Sr1—O4 ⁱⁱ	2.5533 (18)	O3—C5	1.252 (3)
Sr1—O1W	2.5937 (19)	O4—C5	1.267 (3)
Sr1—O3	2.6145 (18)	O4—Sr1 ⁱ	2.5533 (18)
Sr1—O1 ⁱⁱⁱ	2.6155 (18)	C1—C2	1.394 (4)
Sr1—N1	2.714 (2)	C1—C5	1.517 (4)
Sr1—O2 ⁱⁱⁱ	2.8517 (18)	C2—C6	1.516 (4)
Sr1—C6 ⁱⁱⁱ	3.082 (3)	C3—C4	1.381 (4)
Sr1—Sr1 ^{iv}	4.4235 (5)	C3—H3A	0.9500
Sr1—H1W2	2.9292	C4—H4A	0.9500
Sr1—H2W2	2.9320	C6—Sr1 ^v	3.082 (3)
N1—C4	1.332 (3)	O1W—H1W1	0.8500
N1—C1	1.349 (3)	O1W—H2W1	0.8500
N2—C3	1.331 (3)	O2W—H1W2	0.8500
N2—C2	1.343 (3)	O2W—H2W2	0.8500
O1—C6	1.260 (3)	O3W—H1W3	0.8501
O1—Sr1 ^v	2.6155 (18)	O3W—H2W3	0.8499
O2—C6	1.252 (3)		
O2 ⁱ —Sr1—O2W	75.75 (6)	O2 ⁱⁱⁱ —Sr1—H1W2	70.9
O2 ⁱ —Sr1—O4 ⁱⁱ	157.35 (6)	C6 ⁱⁱⁱ —Sr1—H1W2	76.3
O2W—Sr1—O4 ⁱⁱ	85.61 (6)	Sr1 ^{iv} —Sr1—H1W2	78.0
O2 ⁱ —Sr1—O1W	79.88 (6)	O2 ⁱ —Sr1—H2W2	62.3

O2W—Sr1—O1W	142.83 (6)	O2W—Sr1—H2W2	15.6
O4 ⁱⁱ —Sr1—O1W	122.57 (6)	O4 ⁱⁱ —Sr1—H2W2	100.6
O2 ⁱ —Sr1—O3	84.44 (6)	O1W—Sr1—H2W2	128.0
O2W—Sr1—O3	84.19 (6)	O3—Sr1—H2W2	90.9
O4 ⁱⁱ —Sr1—O3	80.93 (6)	O1 ⁱⁱⁱ —Sr1—H2W2	91.2
O1W—Sr1—O3	121.00 (6)	N1—Sr1—H2W2	152.2
O2 ⁱ —Sr1—O1 ⁱⁱⁱ	114.76 (6)	O2 ⁱⁱⁱ —Sr1—H2W2	60.0
O2W—Sr1—O1 ⁱⁱⁱ	92.48 (6)	C6 ⁱⁱⁱ —Sr1—H2W2	76.1
O4 ⁱⁱ —Sr1—O1 ⁱⁱⁱ	78.28 (6)	Sr1 ^{iv} —Sr1—H2W2	54.3
O1W—Sr1—O1 ⁱⁱⁱ	72.81 (6)	H1W2—Sr1—H2W2	28.2
O3—Sr1—O1 ⁱⁱⁱ	159.14 (6)	C4—N1—C1	117.7 (2)
O2 ⁱ —Sr1—N1	112.29 (6)	C4—N1—Sr1	121.46 (17)
O2W—Sr1—N1	142.46 (6)	C1—N1—Sr1	116.91 (16)
O4 ⁱⁱ —Sr1—N1	75.33 (6)	C3—N2—C2	117.5 (2)
O1W—Sr1—N1	73.21 (6)	C6—O1—Sr1 ^v	99.33 (16)
O3—Sr1—N1	61.32 (6)	C6—O2—Sr1 ⁱⁱ	153.65 (17)
O1 ⁱⁱⁱ —Sr1—N1	114.22 (6)	C6—O2—Sr1 ^v	88.36 (15)
O2 ⁱ —Sr1—O2 ⁱⁱⁱ	68.33 (6)	Sr1 ⁱⁱ —O2—Sr1 ^v	111.67 (6)
O2W—Sr1—O2 ⁱⁱⁱ	71.13 (6)	C5—O3—Sr1	124.02 (17)
O4 ⁱⁱ —Sr1—O2 ⁱⁱⁱ	117.81 (5)	C5—O4—Sr1 ⁱ	132.10 (16)
O1W—Sr1—O2 ⁱⁱⁱ	73.99 (5)	N1—C1—C2	120.3 (2)
O3—Sr1—O2 ⁱⁱⁱ	146.69 (6)	N1—C1—C5	115.2 (2)
O1 ⁱⁱⁱ —Sr1—O2 ⁱⁱⁱ	47.66 (5)	C2—C1—C5	124.4 (2)
N1—Sr1—O2 ⁱⁱⁱ	146.41 (6)	N2—C2—C1	121.3 (2)
O2 ⁱ —Sr1—C6 ⁱⁱⁱ	91.29 (7)	N2—C2—C6	114.0 (2)
O2W—Sr1—C6 ⁱⁱⁱ	82.66 (6)	C1—C2—C6	124.4 (2)
O4 ⁱⁱ —Sr1—C6 ⁱⁱⁱ	99.08 (6)	N2—C3—C4	121.4 (3)
O1W—Sr1—C6 ⁱⁱⁱ	70.19 (6)	N2—C3—H3A	119.3
O3—Sr1—C6 ⁱⁱⁱ	166.80 (6)	C4—C3—H3A	119.3
O1 ⁱⁱⁱ —Sr1—C6 ⁱⁱⁱ	23.79 (6)	N1—C4—C3	121.7 (3)
N1—Sr1—C6 ⁱⁱⁱ	131.61 (7)	N1—C4—H4A	119.1
O2 ⁱⁱⁱ —Sr1—C6 ⁱⁱⁱ	23.97 (6)	C3—C4—H4A	119.1
O2 ⁱ —Sr1—Sr1 ^{iv}	36.81 (4)	O3—C5—O4	126.5 (2)
O2W—Sr1—Sr1 ^{iv}	69.70 (4)	O3—C5—C1	116.9 (2)
O4 ⁱⁱ —Sr1—Sr1 ^{iv}	145.08 (4)	O4—C5—C1	116.6 (2)
O1W—Sr1—Sr1 ^{iv}	73.93 (4)	O2—C6—O1	124.1 (2)
O3—Sr1—Sr1 ^{iv}	118.96 (4)	O2—C6—C2	117.4 (2)
O1 ⁱⁱⁱ —Sr1—Sr1 ^{iv}	78.55 (4)	O1—C6—C2	118.3 (2)
N1—Sr1—Sr1 ^{iv}	138.62 (5)	O2—C6—Sr1 ^v	67.67 (14)
O2 ⁱⁱⁱ —Sr1—Sr1 ^{iv}	31.52 (4)	O1—C6—Sr1 ^v	56.88 (13)
C6 ⁱⁱⁱ —Sr1—Sr1 ^{iv}	54.80 (5)	C2—C6—Sr1 ^v	167.25 (17)

supplementary materials

O2 ⁱ —Sr1—H1W2	90.3	Sr1—O1W—H1W1	122.1
O2W—Sr1—H1W2	15.7	Sr1—O1W—H2W1	126.8
O4 ⁱⁱ —Sr1—H1W2	72.9	H1W1—O1W—H2W1	105.9
O1W—Sr1—H1W2	144.7	Sr1—O2W—H1W2	111.4
O3—Sr1—H1W2	91.3	Sr1—O2W—H2W2	111.6
O1 ⁱⁱⁱ —Sr1—H1W2	81.0	H1W2—O2W—H2W2	114.0
N1—Sr1—H1W2	140.8	H1W3—O3W—H2W3	104.9
O2 ⁱ —Sr1—N1—C4	121.4 (2)	C3—N2—C2—C1	-0.7 (4)
O2W—Sr1—N1—C4	-143.01 (19)	C3—N2—C2—C6	-175.0 (2)
O4 ⁱⁱ —Sr1—N1—C4	-81.1 (2)	N1—C1—C2—N2	-0.4 (4)
O1W—Sr1—N1—C4	50.2 (2)	C5—C1—C2—N2	178.5 (2)
O3—Sr1—N1—C4	-168.7 (2)	N1—C1—C2—C6	173.3 (2)
O1 ⁱⁱⁱ —Sr1—N1—C4	-11.5 (2)	C5—C1—C2—C6	-7.8 (4)
O2 ⁱⁱⁱ —Sr1—N1—C4	37.4 (3)	C2—N2—C3—C4	1.3 (4)
C6 ⁱⁱⁱ —Sr1—N1—C4	8.1 (2)	C1—N1—C4—C3	-0.3 (4)
Sr1 ^{iv} —Sr1—N1—C4	89.0 (2)	Sr1—N1—C4—C3	156.5 (2)
O2 ⁱ —Sr1—N1—C1	-81.51 (18)	N2—C3—C4—N1	-0.8 (4)
O2W—Sr1—N1—C1	14.0 (2)	Sr1—O3—C5—O4	-162.37 (19)
O4 ⁱⁱ —Sr1—N1—C1	75.96 (18)	Sr1—O3—C5—C1	17.6 (3)
O1W—Sr1—N1—C1	-152.72 (19)	Sr1 ⁱ —O4—C5—O3	96.7 (3)
O3—Sr1—N1—C1	-11.61 (17)	Sr1 ⁱ —O4—C5—C1	-83.2 (3)
O1 ⁱⁱⁱ —Sr1—N1—C1	145.59 (17)	N1—C1—C5—O3	-27.8 (3)
O2 ⁱⁱⁱ —Sr1—N1—C1	-165.53 (15)	C2—C1—C5—O3	153.3 (3)
C6 ⁱⁱⁱ —Sr1—N1—C1	165.13 (16)	N1—C1—C5—O4	152.2 (2)
Sr1 ^{iv} —Sr1—N1—C1	-113.97 (17)	C2—C1—C5—O4	-26.8 (4)
O2 ⁱ —Sr1—O3—C5	115.1 (2)	Sr1 ⁱⁱ —O2—C6—O1	148.1 (3)
O2W—Sr1—O3—C5	-168.7 (2)	Sr1 ^v —O2—C6—O1	7.3 (3)
O4 ⁱⁱ —Sr1—O3—C5	-82.2 (2)	Sr1 ⁱⁱ —O2—C6—C2	-26.3 (5)
O1W—Sr1—O3—C5	40.4 (2)	Sr1 ^v —O2—C6—C2	-167.1 (2)
O1 ⁱⁱⁱ —Sr1—O3—C5	-87.1 (3)	Sr1 ⁱⁱ —O2—C6—Sr1 ^v	140.8 (4)
N1—Sr1—O3—C5	-4.08 (19)	Sr1 ^v —O1—C6—O2	-8.1 (3)
O2 ⁱⁱⁱ —Sr1—O3—C5	149.62 (18)	Sr1 ^v —O1—C6—C2	166.25 (19)
C6 ⁱⁱⁱ —Sr1—O3—C5	-173.4 (3)	N2—C2—C6—O2	110.2 (3)
Sr1 ^{iv} —Sr1—O3—C5	128.36 (19)	C1—C2—C6—O2	-63.9 (4)
C4—N1—C1—C2	0.9 (4)	N2—C2—C6—O1	-64.5 (3)
Sr1—N1—C1—C2	-157.03 (19)	C1—C2—C6—O1	121.4 (3)
C4—N1—C1—C5	-178.1 (2)	N2—C2—C6—Sr1 ^v	-0.2 (9)
Sr1—N1—C1—C5	24.0 (3)	C1—C2—C6—Sr1 ^v	-174.3 (7)

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

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—H1W1···O3W ⁱ	0.85	1.87	2.713 (3)	170
O1W—H2W1···O3W ^{vi}	0.85	1.90	2.744 (3)	171
O2W—H1W2···O1 ⁱⁱ	0.85	1.85	2.696 (3)	174
O2W—H2W2···O1W ^{iv}	0.85	2.01	2.857 (3)	178
O3W—H1W3···O4	0.85	1.94	2.781 (3)	170
O3W—H2W3···N2 ^{vii}	0.85	1.96	2.792 (3)	168

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

Fig. 1

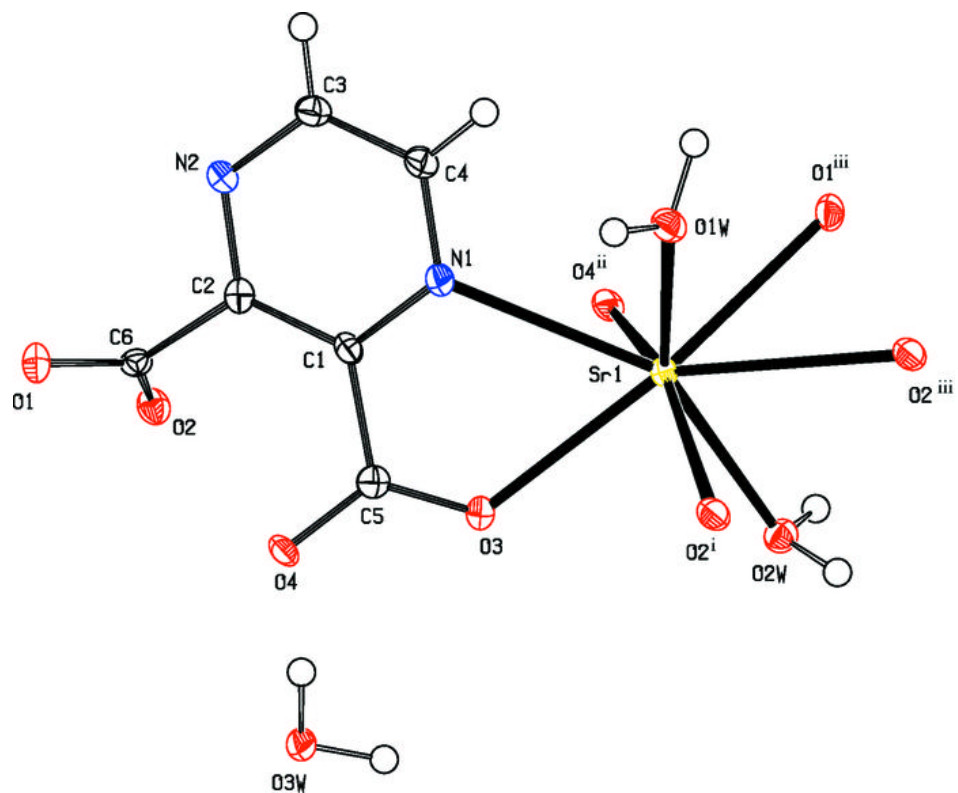


Fig. 2

