

Poly[tetraaqua- μ_3 -pyridine-3,5-dicarboxylato-strontium(II)]

Hossein Aghabozorg,^{a*} Andya Nemati,^a Zohreh Derikvand,^a Mohammad Ghadermazi^b and Shirin Daneshvar^c

^aDepartment of Chemistry, Teacher Training University, 49 Mofateh Avenue, 15614 Tehran, Iran, ^bDepartment of Chemistry, University of Kurdistan, Sanandaj, Iran, and ^cIslamic Azad University, North Tehran Branch, Tehran, Iran
Correspondence e-mail: haghazorg@yahoo.com

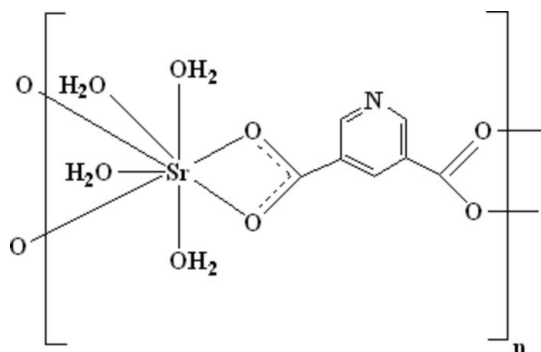
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.029; wR factor = 0.066; data-to-parameter ratio = 16.5.

The reaction of strontium(II) nitrate with the proton-transfer compound (pdaH₂)(py-3,5-dc)·H₂O (where pda = propane-1,3-diamine and py-3,5-dcH₂ = pyridine-3,5-dicarboxylic acid) leads to the formation of the title polymeric compound, [Sr(C₇H₃NO₄)(H₂O)₄]_n. The propane-1,3-diaminium cation is not incorporated in this crystal structure. The Sr^{II} atom lies on an inversion centre and is eight-coordinated by four O atoms from three py-3,5-dc ligands and four O atoms from four coordinated water molecules. The coordination polyhedron of the Sr^{II} atom is a distorted dodecahedron. These binuclear units are connected *via* the carboxylate O atoms to build a one-dimensional polymeric chain. In the crystal structure, non-covalent interactions consisting of hydrogen bonds ($X\cdots H\cdots O$, with $X = O$ and C) and π - π stacking interactions [3.4604 (19) Å] connect the various components to form a supramolecular structure.

Related literature

For related literature, see: Aghabozorg *et al.* (2006, 2007, 2008); Starosta *et al.* (2002a,b).



Experimental

Crystal data

[Sr(C₇H₃NO₄)(H₂O)₄]
 $M_r = 324.79$
 Triclinic, $P\bar{1}$
 $a = 7.066$ (2) Å
 $b = 8.308$ (3) Å
 $c = 10.368$ (3) Å
 $\alpha = 69.405$ (6)°
 $\beta = 72.144$ (6)°
 $\gamma = 75.944$ (6)°
 $V = 536.0$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 5.06$ mm⁻¹
 $T = 100$ (2) K
 $0.30 \times 0.22 \times 0.18$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (APEX2; Bruker, 2005)
 $T_{\min} = 0.257$, $T_{\max} = 0.402$
 4533 measured reflections
 2540 independent reflections
 2277 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.065$
 $S = 0.99$
 2540 reflections
 154 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.66$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA \cdots O3 ⁱⁱⁱ	0.83	1.92	2.744 (3)	178
O1W—H1WB \cdots O3 ⁱⁱⁱ	0.92	1.85	2.754 (3)	168
O2W—H2WA \cdots O4 ⁱⁱⁱ	0.86	1.90	2.747 (3)	169
O2W—H2WB \cdots O4 ⁱ	0.86	1.98	2.816 (3)	162
O3W—H3WA \cdots O4 ^{iv}	0.93	1.95	2.863 (3)	168
O3W—H3WB \cdots O4W ⁱⁱ	0.85	2.31	3.159 (4)	175
O4W—H4WA \cdots N1 ^v	0.83	1.92	2.739 (4)	169
O4W—H4WB \cdots O4 ^{vi}	0.79	2.42	3.192 (4)	164
C3—H3A \cdots O1W ⁱⁱ	0.95	2.40	3.324 (4)	164

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

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: APEX2; 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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2030).

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supplementary materials

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Poly[tetraaqua- μ_3 -pyridine-3,5-dicarboxylato-strontium(II)]

H. Aghabozorg, A. Nemati, Z. Derikvand, M. Ghadermazi and S. Daneshvar

Comment

We have previously reported a proton transfer system, prepared using pyridine-3,5-dicarboxylic acid and propane-1,3-diamine (pdaH₂)(py-3,5-dc).H₂O (Aghabozorg *et al.* 2006; Aghabozorg *et al.*, 2007). Pyridine-3,5-dicarboxylic acid is an interesting ligand because it is highly symmetrical, potentially multidentate and it can participate in hydrogen bonding interactions with N and O acceptors. It may also exhibit π - π interactions (Starosta *et al.*, 2002a,b) and some polymeric Cd(II) complexes of this ligand have been published. Here we report on the crystal structure of the title polymeric compound, (I).

The compound (I) is a centrosymmetric polymer (Fig. 1). The Sr—O distances are in the range of 2.5240 (19)–2.7395 (18) Å, and the summation of the bond angles around of Sr^{II} atom is equal to 359.24°, indicating that the Sr^{II} atom is located in the center of the plane (O2ⁱ, O4W, O1ⁱⁱ, O3W, O2W). This shows that it has a distorted dodecahedral geometry (Fig. 2).

The carboxylate groups from the py-3,5-dc ligands link two Sr^{II} centers by two O1 atoms or two O2 atoms alternatively to form binuclear units and this results in the formation of a one-dimensional polymer chain. Each of the atoms, O1 and O2, from the py-3,5-dc ligands are connected to two Sr^{II} atoms, but only atoms O3, O4 and N1 from these ligands build hydrogen bonds with the coordinated water molecules. There are a large number of O—H \cdots O, N—H \cdots O and C—H \cdots O hydrogen bonds with distances ranging from 2.739 (4) to 3.324 (4) Å (Table 2 and Fig. 3).

In the crystal structure of (I), noncovalent interactions consisting of hydrogen bonds, π - π stacking interactions of 3.4604 (19) Å between Cg1 and Cg1ⁱ (Fig. 4 and Table 1) [Cg1 is centroid of ring N1/C1–C5; symmetry code: (i) = -x, 1 - y, 2 - z] connect the various components to form the supramolecular structure.

Experimental

Compound (I) was prepared by the reaction of (pdaH₂)(py-3,5-dc).H₂O (241.0 mg, 1.0 mmol) [Aghabozorg *et al.*, 2006], in water (20 ml) with Sr(NO₃)₂ (105.8 mg, 0.5 mmol) in water (20 ml), in a 2:1 molar ratio. Colorless crystals were obtained by slow evaporation of the solvent at room temperature.

Refinement

All hydrogen atoms were located in difference Fourier maps. The water H-atoms were treated as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{O})$; O—H = 0.7018–0.9275 Å. The C-bound H-atoms were included in calculated positions and treated as riding atoms with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Figures

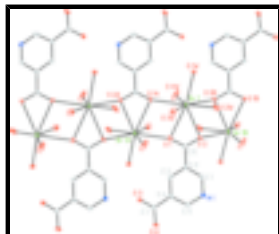


Fig. 1. Molecular structure of compound (I), with displacement ellipsoids drawn at the 50% probability level [H-atoms have been omitted for clarity; symmetry codes: A = $-x, 1 - y, 1 - z$ and B = $1 - x, 1 - y, 1 - z$].

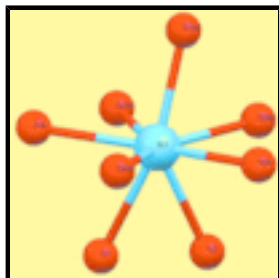


Fig. 2. A view of the distorted dodecahedral environment around the Sr^{II} atom.

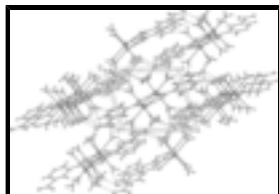


Fig. 3. A view along the *a* axis of the crystal packing of compound (I). Hydrogen bonds are shown as dashed lines.

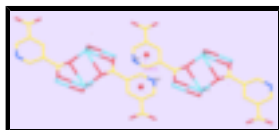


Fig. 4. π - π stacking interactions ($Cg1-Cg1^i$) in compound (I) [$Cg1$: N1/C1-C5; symmetry code: (i) = $-x, 1 - y, 2 - z$].

Poly[tetraaqua- μ_3 -pyridine-3,5-dicarboxylato-strontium(II)]

Crystal data

[Sr(C₇H₃NO₄)(H₂O)₄]

$M_r = 324.79$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.066$ (2) Å

$b = 8.308$ (3) Å

$c = 10.368$ (3) Å

$\alpha = 69.405$ (6)°

$\beta = 72.144$ (6)°

$\gamma = 75.944$ (6)°

$V = 536.0$ (3) Å³

$Z = 2$

$F_{000} = 324$

$D_x = 2.012$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2708 reflections

$\theta = 2.6-30.0^\circ$

$\mu = 5.06$ mm⁻¹

$T = 100$ (2) K

Prism, colourless

$0.30 \times 0.22 \times 0.18$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer	2540 independent reflections
Radiation source: fine-focus sealed tube	2277 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.038$
$T = 100(2)$ K	$\theta_{\text{max}} = 28.0^\circ$
ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -8 \rightarrow 9$
$T_{\text{min}} = 0.257$, $T_{\text{max}} = 0.402$	$k = -10 \rightarrow 10$
4533 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
2540 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
154 parameters	$\Delta\rho_{\text{max}} = 0.65 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.66 \text{ e } \text{\AA}^{-3}$
	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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.27281 (3)	0.61146 (3)	0.39986 (2)	0.00977 (8)
O1	0.0595 (3)	0.4107 (2)	0.64828 (18)	0.0145 (4)
O2	0.3414 (3)	0.4771 (2)	0.65401 (17)	0.0134 (4)
O3	-0.3603 (3)	0.0688 (3)	1.10676 (18)	0.0171 (4)
O4	-0.2944 (3)	0.0464 (3)	1.30871 (19)	0.0208 (4)
N1	0.1904 (3)	0.3128 (3)	1.0958 (2)	0.0117 (4)

supplementary materials

C1	0.2362 (4)	0.3684 (3)	0.9544 (3)	0.0106 (5)
H1A	0.3469	0.4306	0.9064	0.013*
C2	0.1298 (4)	0.3398 (3)	0.8736 (2)	0.0098 (5)
C3	-0.0306 (4)	0.2479 (3)	0.9450 (2)	0.0110 (5)
H3A	-0.1061	0.2257	0.8931	0.013*
C4	-0.0808 (4)	0.1885 (3)	1.0922 (3)	0.0106 (5)
C5	0.0352 (4)	0.2248 (3)	1.1627 (3)	0.0120 (5)
H5A	0.0023	0.1849	1.2635	0.014*
C6	0.1813 (4)	0.4129 (3)	0.7142 (2)	0.0103 (5)
C7	-0.2567 (4)	0.0930 (3)	1.1741 (3)	0.0115 (5)
O1W	0.3572 (3)	0.8563 (2)	0.17360 (18)	0.0157 (4)
H1WA	0.3591	0.8811	0.0888	0.019*
H1WB	0.4416	0.9316	0.1631	0.019*
O2W	0.4291 (3)	0.8227 (3)	0.4569 (2)	0.0253 (5)
H2WA	0.5046	0.8998	0.4043	0.030*
H2WB	0.3802	0.8404	0.5389	0.030*
O3W	-0.0230 (3)	0.8411 (3)	0.4823 (2)	0.0223 (4)
H3WA	-0.1078	0.8936	0.4213	0.027*
H3WB	-0.1145	0.7842	0.5417	0.027*
O4W	0.3526 (3)	0.3705 (3)	0.2812 (3)	0.0372 (6)
H4WA	0.3192	0.3499	0.2194	0.045*
H4WB	0.4424	0.2960	0.3008	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00856 (13)	0.01397 (13)	0.00712 (11)	-0.00508 (8)	-0.00166 (8)	-0.00157 (8)
O1	0.0111 (9)	0.0211 (11)	0.0115 (8)	-0.0067 (7)	-0.0042 (7)	-0.0012 (7)
O2	0.0096 (9)	0.0179 (10)	0.0100 (8)	-0.0065 (7)	-0.0011 (7)	0.0008 (7)
O3	0.0166 (10)	0.0243 (11)	0.0120 (8)	-0.0116 (8)	-0.0025 (7)	-0.0026 (8)
O4	0.0223 (11)	0.0316 (13)	0.0097 (8)	-0.0172 (9)	0.0009 (8)	-0.0028 (8)
N1	0.0117 (11)	0.0117 (11)	0.0117 (10)	-0.0014 (8)	-0.0038 (8)	-0.0028 (8)
C1	0.0089 (12)	0.0102 (13)	0.0122 (11)	-0.0021 (9)	-0.0020 (9)	-0.0029 (10)
C2	0.0083 (12)	0.0095 (13)	0.0095 (11)	0.0004 (9)	-0.0023 (9)	-0.0013 (9)
C3	0.0105 (12)	0.0109 (13)	0.0111 (11)	-0.0005 (10)	-0.0040 (9)	-0.0021 (9)
C4	0.0100 (12)	0.0089 (13)	0.0110 (11)	-0.0026 (9)	-0.0010 (9)	-0.0011 (9)
C5	0.0138 (13)	0.0108 (13)	0.0096 (11)	-0.0019 (10)	-0.0016 (9)	-0.0020 (9)
C6	0.0107 (12)	0.0085 (13)	0.0104 (11)	-0.0011 (9)	-0.0021 (9)	-0.0018 (9)
C7	0.0112 (13)	0.0112 (13)	0.0112 (11)	-0.0022 (10)	-0.0008 (9)	-0.0034 (10)
O1W	0.0186 (10)	0.0179 (10)	0.0109 (8)	-0.0100 (8)	-0.0046 (7)	0.0010 (7)
O2W	0.0307 (12)	0.0316 (13)	0.0181 (10)	-0.0236 (10)	0.0068 (9)	-0.0110 (9)
O3W	0.0261 (11)	0.0217 (12)	0.0211 (10)	-0.0013 (9)	-0.0091 (8)	-0.0077 (9)
O4W	0.0324 (13)	0.0473 (16)	0.0527 (15)	0.0211 (11)	-0.0306 (11)	-0.0405 (13)

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

Sr1—O1W	2.5240 (19)	C1—C2	1.392 (3)
Sr1—O4W	2.568 (2)	C1—H1A	0.9500

Sr1—O2 ⁱ	2.5816 (19)	C2—C3	1.387 (3)
Sr1—O2W	2.592 (2)	C2—C6	1.505 (3)
Sr1—O1 ⁱⁱ	2.6063 (19)	C3—C4	1.386 (3)
Sr1—O3W	2.618 (2)	C3—H3A	0.9500
Sr1—O2	2.6223 (19)	C4—C5	1.393 (3)
Sr1—O1	2.7395 (18)	C4—C7	1.501 (3)
Sr1—C6	3.034 (3)	C5—H5A	0.9500
Sr1—Sr1 ⁱ	4.0677 (11)	O1W—H1WA	0.8258
Sr1—Sr1 ⁱⁱ	4.2965 (12)	O1W—H1WB	0.9233
O1—C6	1.259 (3)	O2W—H2WA	0.8569
O1—Sr1 ⁱⁱ	2.6063 (19)	O2W—H2WB	0.8650
O2—C6	1.257 (3)	O3W—H3WA	0.9275
O2—Sr1 ⁱ	2.5816 (19)	O3W—H3WB	0.8485
O3—C7	1.244 (3)	O4W—H4WA	0.8287
O4—C7	1.269 (3)	O4W—H4WB	0.7918
N1—C1	1.332 (3)	Cg1—Cg1(N1/C1-C5) ⁱⁱⁱ	3.4604 (19)
N1—C5	1.335 (3)		
O1W—Sr1—O4W	96.37 (8)	O1 ⁱⁱ —Sr1—Sr1 ⁱⁱ	37.58 (4)
O1W—Sr1—O2 ⁱ	82.73 (6)	O3W—Sr1—Sr1 ⁱⁱ	69.44 (5)
O4W—Sr1—O2 ⁱ	73.73 (6)	O2—Sr1—Sr1 ⁱⁱ	84.10 (4)
O1W—Sr1—O2W	72.85 (7)	O1—Sr1—Sr1 ⁱⁱ	35.47 (4)
O4W—Sr1—O2W	144.24 (7)	C6—Sr1—Sr1 ⁱⁱ	59.79 (5)
O2 ⁱ —Sr1—O2W	71.15 (7)	Sr1 ⁱ —Sr1—Sr1 ⁱⁱ	115.28 (2)
O1W—Sr1—O1 ⁱⁱ	93.47 (6)	C6—O1—Sr1 ⁱⁱ	160.12 (16)
O4W—Sr1—O1 ⁱⁱ	72.57 (6)	C6—O1—Sr1	90.96 (15)
O2 ⁱ —Sr1—O1 ⁱⁱ	145.42 (6)	Sr1 ⁱⁱ —O1—Sr1	106.95 (6)
O2W—Sr1—O1 ⁱⁱ	140.38 (7)	C6—O2—Sr1 ⁱ	141.33 (16)
O1W—Sr1—O3W	85.06 (7)	C6—O2—Sr1	96.51 (14)
O4W—Sr1—O3W	141.51 (7)	Sr1 ⁱ —O2—Sr1	102.83 (6)
O2 ⁱ —Sr1—O3W	143.96 (6)	C1—N1—C5	118.1 (2)
O2W—Sr1—O3W	72.86 (7)	N1—C1—C2	123.1 (2)
O1 ⁱⁱ —Sr1—O3W	68.96 (6)	N1—C1—H1A	118.4
O1W—Sr1—O2	141.03 (6)	C2—C1—H1A	118.4
O4W—Sr1—O2	109.25 (7)	C3—C2—C1	117.8 (2)
O2 ⁱ —Sr1—O2	77.17 (6)	C3—C2—C6	121.0 (2)
O2W—Sr1—O2	69.18 (6)	C1—C2—C6	121.1 (2)
O1 ⁱⁱ —Sr1—O2	121.59 (5)	C4—C3—C2	120.0 (2)
O3W—Sr1—O2	91.91 (6)	C4—C3—H3A	120.0
O1W—Sr1—O1	161.19 (6)	C2—C3—H3A	120.0
O4W—Sr1—O1	92.07 (8)	C3—C4—C5	117.5 (2)
O2 ⁱ —Sr1—O1	115.84 (6)	C3—C4—C7	121.9 (2)
O2W—Sr1—O1	109.03 (6)	C5—C4—C7	120.6 (2)
O1 ⁱⁱ —Sr1—O1	73.05 (6)	N1—C5—C4	123.4 (2)
O3W—Sr1—O1	77.93 (6)	N1—C5—H5A	118.3

supplementary materials

O2—Sr1—O1	48.73 (5)	C4—C5—H5A	118.3
O1W—Sr1—C6	159.89 (7)	O2—C6—O1	123.3 (2)
O4W—Sr1—C6	103.03 (8)	O2—C6—C2	118.2 (2)
O2 ⁱ —Sr1—C6	97.56 (6)	O1—C6—C2	118.4 (2)
O2W—Sr1—C6	88.14 (7)	O2—C6—Sr1	59.18 (12)
O1 ⁱⁱ —Sr1—C6	97.29 (6)	O1—C6—Sr1	64.53 (13)
O3W—Sr1—C6	83.05 (7)	C2—C6—Sr1	171.70 (17)
O2—Sr1—C6	24.31 (6)	O3—C7—O4	123.8 (2)
O1—Sr1—C6	24.51 (6)	O3—C7—C4	118.4 (2)
O1W—Sr1—Sr1 ⁱ	114.89 (5)	O4—C7—C4	117.7 (2)
O4W—Sr1—Sr1 ⁱ	91.99 (5)	Sr1—O1W—H1WA	138.3
O2 ⁱ —Sr1—Sr1 ⁱ	38.94 (4)	Sr1—O1W—H1WB	121.7
O2W—Sr1—Sr1 ⁱ	64.27 (5)	H1WA—O1W—H1WB	97.4
O1 ⁱⁱ —Sr1—Sr1 ⁱ	149.34 (4)	Sr1—O2W—H2WA	132.5
O3W—Sr1—Sr1 ⁱ	122.32 (5)	Sr1—O2W—H2WB	118.0
O2—Sr1—Sr1 ⁱ	38.23 (4)	H2WA—O2W—H2WB	107.9
O1—Sr1—Sr1 ⁱ	81.46 (4)	Sr1—O3W—H3WA	114.3
C6—Sr1—Sr1 ⁱ	59.74 (5)	Sr1—O3W—H3WB	106.3
O1W—Sr1—Sr1 ⁱⁱ	129.81 (4)	H3WA—O3W—H3WB	89.7
O4W—Sr1—Sr1 ⁱⁱ	80.87 (6)	Sr1—O4W—H4WA	138.5
O2 ⁱ —Sr1—Sr1 ⁱⁱ	141.02 (4)	Sr1—O4W—H4WB	115.5
O2W—Sr1—Sr1 ⁱⁱ	132.47 (5)	H4WA—O4W—H4WB	105.6
O1W—Sr1—O1—C6	-125.5 (2)	C2—C3—C4—C5	0.0 (4)
O4W—Sr1—O1—C6	117.69 (15)	C2—C3—C4—C7	178.2 (2)
O2 ⁱ —Sr1—O1—C6	44.79 (16)	C1—N1—C5—C4	0.0 (4)
O2W—Sr1—O1—C6	-32.93 (16)	C3—C4—C5—N1	-0.1 (4)
O1 ⁱⁱ —Sr1—O1—C6	-171.24 (19)	C7—C4—C5—N1	-178.3 (2)
O3W—Sr1—O1—C6	-99.82 (16)	Sr1 ⁱ —O2—C6—O1	-112.8 (3)
O2—Sr1—O1—C6	3.66 (14)	Sr1—O2—C6—O1	7.2 (3)
Sr1 ⁱ —Sr1—O1—C6	25.99 (14)	Sr1 ⁱ —O2—C6—C2	69.0 (3)
Sr1 ⁱⁱ —Sr1—O1—C6	-171.24 (19)	Sr1—O2—C6—C2	-170.94 (19)
O1W—Sr1—O1—Sr1 ⁱⁱ	45.7 (2)	Sr1 ⁱ —O2—C6—Sr1	-120.0 (2)
O4W—Sr1—O1—Sr1 ⁱⁱ	-71.07 (7)	Sr1 ⁱⁱ —O1—C6—O2	-161.5 (4)
O2 ⁱ —Sr1—O1—Sr1 ⁱⁱ	-143.98 (6)	Sr1—O1—C6—O2	-6.9 (3)
O2W—Sr1—O1—Sr1 ⁱⁱ	138.31 (7)	Sr1 ⁱⁱ —O1—C6—C2	16.7 (7)
O1 ⁱⁱ —Sr1—O1—Sr1 ⁱⁱ	0.0	Sr1—O1—C6—C2	171.3 (2)
O3W—Sr1—O1—Sr1 ⁱⁱ	71.42 (7)	Sr1 ⁱⁱ —O1—C6—Sr1	-154.6 (5)
O2—Sr1—O1—Sr1 ⁱⁱ	174.89 (11)	C3—C2—C6—O2	-171.8 (2)
C6—Sr1—O1—Sr1 ⁱⁱ	171.24 (19)	C1—C2—C6—O2	10.9 (4)
Sr1 ⁱ —Sr1—O1—Sr1 ⁱⁱ	-162.78 (6)	C3—C2—C6—O1	9.9 (4)
O1W—Sr1—O2—C6	152.90 (14)	C1—C2—C6—O1	-167.3 (2)
O4W—Sr1—O2—C6	-78.87 (16)	O1W—Sr1—C6—O2	-56.4 (2)
O2 ⁱ —Sr1—O2—C6	-146.30 (18)	O4W—Sr1—C6—O2	108.05 (15)

O2W—Sr1—O2—C6	139.24 (16)	O2 ⁱ —Sr1—C6—O2	33.08 (18)
O1 ⁱⁱ —Sr1—O2—C6	2.05 (17)	O2W—Sr1—C6—O2	-37.63 (15)
O3W—Sr1—O2—C6	68.40 (15)	O1 ⁱⁱ —Sr1—C6—O2	-178.24 (15)
O1—Sr1—O2—C6	-3.68 (14)	O3W—Sr1—C6—O2	-110.59 (15)
Sr1 ⁱ —Sr1—O2—C6	-146.30 (18)	O1—Sr1—C6—O2	173.3 (2)
Sr1 ⁱⁱ —Sr1—O2—C6	-0.71 (14)	Sr1 ⁱ —Sr1—C6—O2	23.42 (13)
O1W—Sr1—O2—Sr1 ⁱ	-60.80 (11)	Sr1 ⁱⁱ —Sr1—C6—O2	179.19 (16)
O4W—Sr1—O2—Sr1 ⁱ	67.43 (8)	O1W—Sr1—C6—O1	130.25 (19)
O2 ⁱ —Sr1—O2—Sr1 ⁱ	0.0	O4W—Sr1—C6—O1	-65.27 (16)
O2W—Sr1—O2—Sr1 ⁱ	-74.46 (7)	O2 ⁱ —Sr1—C6—O1	-140.24 (15)
O1 ⁱⁱ —Sr1—O2—Sr1 ⁱ	148.35 (6)	O2W—Sr1—C6—O1	149.06 (15)
O3W—Sr1—O2—Sr1 ⁱ	-145.30 (7)	O1 ⁱⁱ —Sr1—C6—O1	8.45 (18)
O1—Sr1—O2—Sr1 ⁱ	142.62 (10)	O3W—Sr1—C6—O1	76.10 (15)
C6—Sr1—O2—Sr1 ⁱ	146.30 (18)	O2—Sr1—C6—O1	-173.3 (2)
Sr1 ⁱⁱ —Sr1—O2—Sr1 ⁱ	145.59 (6)	Sr1 ⁱ —Sr1—C6—O1	-149.89 (16)
C5—N1—C1—C2	0.3 (4)	Sr1 ⁱⁱ —Sr1—C6—O1	5.87 (12)
N1—C1—C2—C3	-0.4 (4)	C3—C4—C7—O3	-0.7 (4)
N1—C1—C2—C6	177.0 (2)	C5—C4—C7—O3	177.5 (2)
C1—C2—C3—C4	0.2 (4)	C3—C4—C7—O4	-178.6 (2)
C6—C2—C3—C4	-177.1 (2)	C5—C4—C7—O4	-0.4 (4)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H1WA \cdots O3 ⁱⁱ	0.83	1.92	2.744 (3)	178
O1W—H1WB \cdots O3 ^{iv}	0.92	1.85	2.754 (3)	168
O2W—H2WA \cdots O4 ^{iv}	0.86	1.90	2.747 (3)	169
O2W—H2WB \cdots O4 ⁱⁱⁱ	0.86	1.98	2.816 (3)	162
O3W—H3WA \cdots O4 ^v	0.93	1.95	2.863 (3)	168
O3W—H3WB \cdots O4W ⁱⁱ	0.85	2.31	3.159 (4)	175
O4W—H4WA \cdots N1 ^{vi}	0.83	1.92	2.739 (4)	169
O4W—H4WB \cdots O4 ^{vii}	0.79	2.42	3.192 (4)	164
C3—H3A \cdots O1W ⁱⁱ	0.95	2.40	3.324 (4)	164

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

Fig. 2

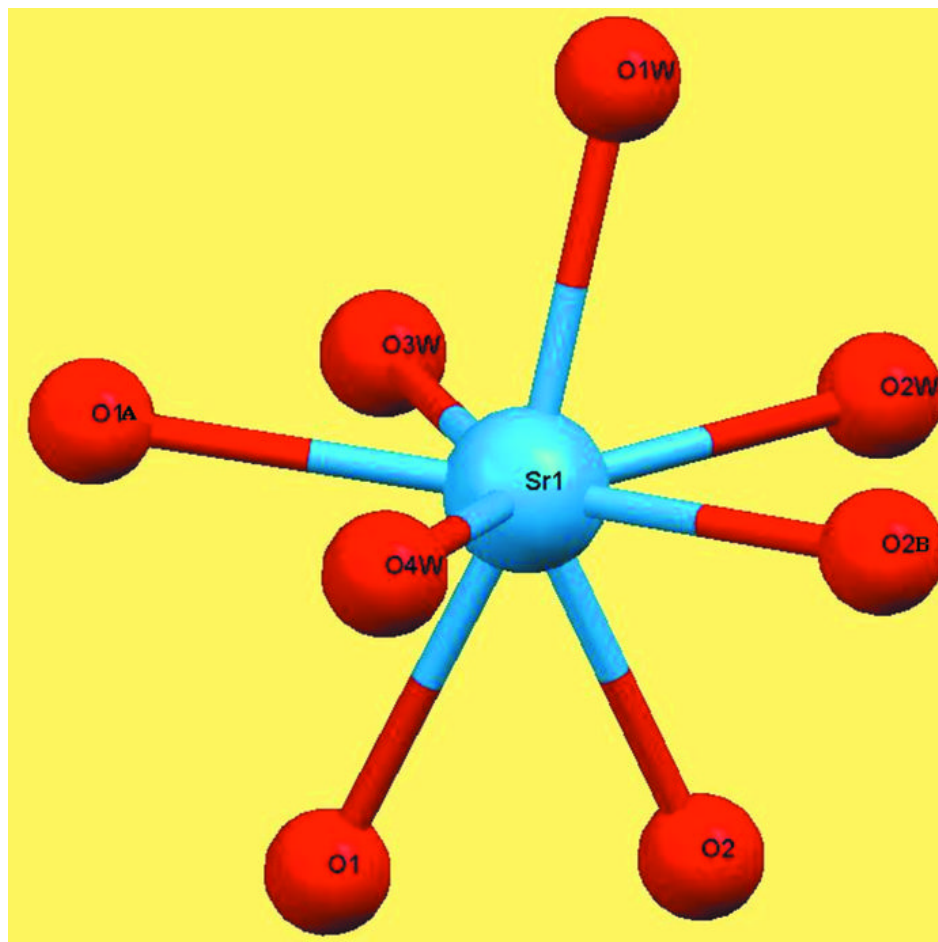


Fig. 3

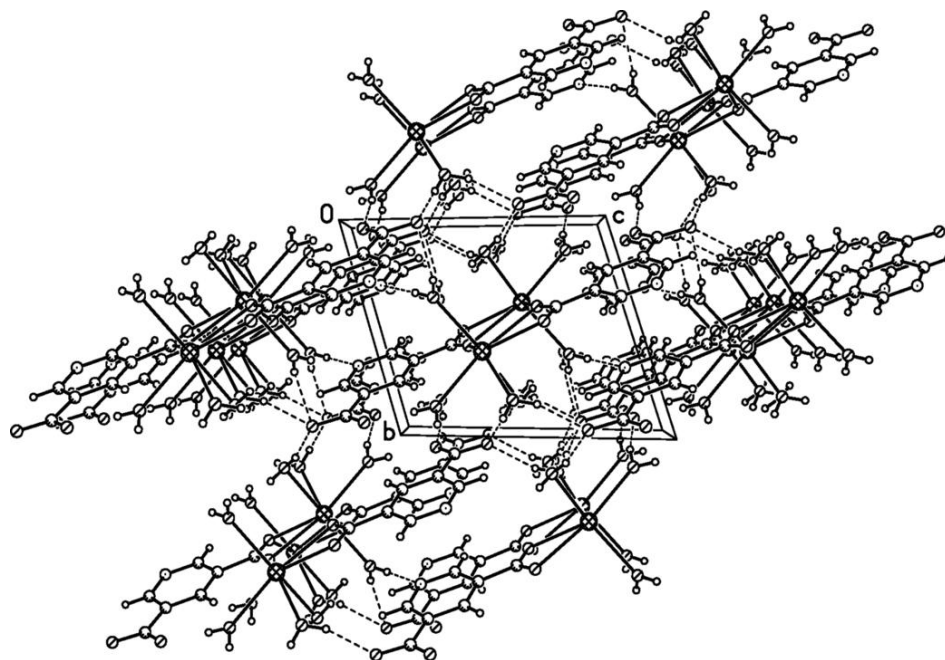


Fig. 4

