

catena-Poly[[aqua(*N,N*-dimethylformamide- κ O)strontium(II)]-bis[μ -2-(4-carboxyphenoxy)propionato- κ^3 O,O':O']]

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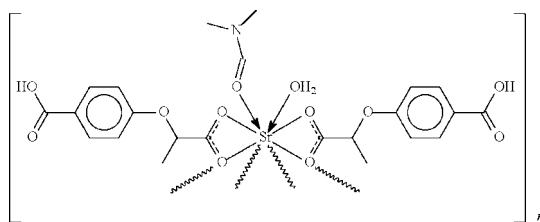
Received 17 October 2007; accepted 21 October 2007

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.006$ Å; disorder in main residue; R factor = 0.059; wR factor = 0.183; data-to-parameter ratio = 15.2.

In the crystal structure of the polymeric title compound, $[Sr(C_{10}H_9O_5)_2(C_3H_7NO)(H_2O)]_n$, the Sr^{II} atom is O,O' -chelated by the carboxylate end of two 2-(4-carboxyphenoxy)propionate monoanions, and is coordinated by a water molecule and a dimethylformamide (DMF) molecule. It also interacts with the carboxylate O atom of two adjacent monoanions; these bonds give rise to a zigzag chain along the a axis. Meanwhile, the carboxyl $-CO_2H$ end of the anion interacts with an acceptor site [$O \cdots O = 2.629$ (4) Å]; this interaction and hydrogen bonding involving the water molecule [$O \cdots O = 3.191$ (5) Å] give rise to a three-dimensional network. The eight coordinating O atoms comprise an irregular polyhedron around the metal atom. The Sr atom, the water O atom, and the N and O atoms of the DMF molecule lie on a special position of site symmetry m ; the DMF molecule is disordered about the mirror plane.

Related literature

For transition metal derivatives of 2-[4-(carboxyphenoxy)propionic acid, see: Deng *et al.* (2007a,b); Xiao *et al.* (2007).



Experimental

Crystal data

$[Sr(C_{10}H_9O_5)_2(C_3H_7NO)(H_2O)]$	$V = 2499.17$ (17) Å ³
$M_r = 597.08$	$Z = 4$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
$a = 7.8303$ (3) Å	$\mu = 2.22$ mm ⁻¹
$b = 23.973$ (1) Å	$T = 295$ (2) K
$c = 13.3136$ (5) Å	$0.30 \times 0.24 \times 0.18$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	36357 measured reflections
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	2917 independent reflections
$(ABSCOR; Higashi, 1995)$	2218 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.087$	$R_{\text{int}} = 0.087$
$T_{\min} = 0.443$, $T_{\max} = 0.690$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$	192 parameters
$wR(F^2) = 0.183$	H-atom parameters constrained
$S = 1.17$	$\Delta\rho_{\max} = 2.43$ e Å ⁻³
2917 reflections	$\Delta\rho_{\min} = -1.17$ e Å ⁻³

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H5O \cdots O1 ⁱ	0.82	1.81	2.629 (4)	174
O1W—H1W \cdots O4 ⁱⁱ	0.82	2.37	3.191 (5)	178

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

The authors thank the Heilongjiang Province Natural Science Foundation (grant No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (grant No. 1054 G036), Heilongjiang University and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2486).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
- Deng, Z.-P., Gao, S. & Chen, P.-G. (2007a). *Acta Cryst. E* **63**, m296–m298.
- Deng, Z.-P., Gao, S. & Chen, P.-G. (2007b). *Acta Cryst. E* **63**, m553–m554.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Westrip, S. P. (2007). *publCIF*. In preparation.
- Xiao, Y.-H., Kong, L.-L. & Gao, S. (2007). *Acta Cryst. E* **63**, m1587–m1588.

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Acta Cryst. (2007). E63, m2849 [doi:10.1107/S1600536807052166]

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L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Comment

This report continues previous studies on the transition metal derivatives of 2-[4-carboxylatophenoxy]propionic acid (Deng *et al.*, 2007a,b; Xiao *et al.*, 2007). The studies are extended to the main-group metal derivatives. In the present strontium compound (Fig. 1), the metal shows irregular eight-coordination (Fig. 2).

Experimental

A solution of strontium carbonate (1 mmol) was added to a solution of 2-(4-carboxylatophenoxy)propionic acid (1 mmol) in DMF. The mixture was filtered and colourless were isolated after several days.

Refinement

Carbon- and oxygen-bound H atoms were placed in calculated positions [$C-H = 0.93-0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2-1.5 U_{\text{eq}}(\text{C})$; $O-H = 0.82 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$], and were included in the refinement in the riding-model approximation. A rotating group model was used for the methyl and hydroxyl groups. The final difference Fourier map had large peaks/holes in the vicinity of the strontium atom.

Figures

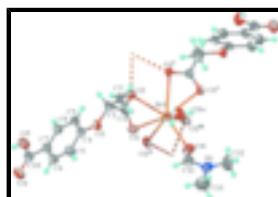


Fig. 1. Part of the polymeric structure of the title compound, showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Symmetry codes: (i) $x, 3/2 - y, z$; (ii) $1/2 + x, 3/2 - y, 1/2 - z$; (iii) $1/2 + x, y, 1/2 - z$.

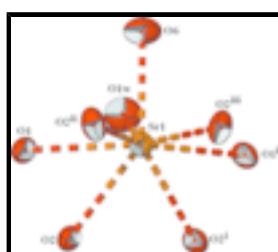


Fig. 2. Irregular eight-coordinate geometry of Sr.

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Crystal data

[Sr(C ₁₀ H ₉ O ₅) ₂ (C ₃ H ₇ NO)(H ₂ O)]	$F_{000} = 1224$
$M_r = 597.08$	$D_x = 1.587 \text{ Mg m}^{-3}$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
Hall symbol: -P 2ac 2n	$\lambda = 0.71073 \text{ \AA}$
$a = 7.8303 (3) \text{ \AA}$	Cell parameters from 21767 reflections
$b = 23.973 (1) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$c = 13.3136 (5) \text{ \AA}$	$\mu = 2.22 \text{ mm}^{-1}$
$V = 2499.17 (17) \text{ \AA}^3$	$T = 295 (2) \text{ K}$
$Z = 4$	Prism, colourless
	$0.30 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	2917 independent reflections
Radiation source: fine-focus sealed tube	2218 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.087$
Detector resolution: 10.000 pixels mm ⁻¹	$\theta_{\text{max}} = 27.5^\circ$
$T = 295(2) \text{ K}$	$\theta_{\text{min}} = 3.0^\circ$
ω scans	$h = -10 \rightarrow 9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -31 \rightarrow 31$
$T_{\text{min}} = 0.443$, $T_{\text{max}} = 0.690$	$l = -17 \rightarrow 17$
36357 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.059$	$w = 1/[\sigma^2(F_o^2) + (0.1071P)^2 + 0.6055P]$
	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.183$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.17$	$\Delta\rho_{\text{max}} = 2.43 \text{ e \AA}^{-3}$
2917 reflections	$\Delta\rho_{\text{min}} = -1.17 \text{ e \AA}^{-3}$
192 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.009 (2)
Secondary atom site location: difference Fourier map	

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sr1	0.29520 (6)	0.7500	0.32490 (4)	0.0362 (3)	
O1	0.1965 (3)	0.64729 (13)	0.3671 (3)	0.0451 (7)	
O2	0.0140 (4)	0.69144 (12)	0.2698 (2)	0.0495 (8)	
O3	-0.0257 (4)	0.55897 (11)	0.3874 (2)	0.0433 (7)	
O4	0.2868 (5)	0.36228 (16)	0.1218 (3)	0.0652 (10)	
O5	0.1929 (4)	0.42171 (16)	0.0062 (3)	0.0608 (10)	
H5o	0.2231	0.4013	-0.0400	0.091*	
O6	0.5137 (6)	0.7500	0.4629 (4)	0.0636 (13)	
O1W	0.1315 (8)	0.7500	0.5024 (4)	0.0707 (14)	
H1W	0.1512	0.7793	0.5320	0.106*	
N1	0.5613 (8)	0.7500	0.6316 (4)	0.0585 (15)	
C1	0.0504 (5)	0.65244 (17)	0.3291 (3)	0.0371 (9)	
C2	-0.0920 (5)	0.61218 (17)	0.3582 (3)	0.0425 (9)	
H2	-0.1719	0.6077	0.3021	0.051*	
C3	-0.1852 (6)	0.6352 (2)	0.4494 (4)	0.0587 (13)	
H3A	-0.2794	0.6113	0.4658	0.088*	
H3B	-0.2270	0.6720	0.4346	0.088*	
H3C	-0.1080	0.6370	0.5053	0.088*	
C4	0.0337 (5)	0.52473 (17)	0.3125 (3)	0.0402 (9)	
C5	0.1010 (6)	0.47397 (18)	0.3454 (3)	0.0492 (10)	
H5	0.1054	0.4658	0.4136	0.059*	
C6	0.1603 (6)	0.43628 (18)	0.2766 (4)	0.0501 (11)	
H6	0.2052	0.4025	0.2988	0.060*	
C7	0.1548 (6)	0.44757 (19)	0.1737 (3)	0.0449 (10)	
C8	0.0878 (6)	0.49822 (18)	0.1425 (4)	0.0456 (9)	
H8	0.0829	0.5063	0.0742	0.055*	
C9	0.0280 (6)	0.53707 (18)	0.2114 (4)	0.0448 (10)	
H9	-0.0155	0.5711	0.1896	0.054*	
C10	0.2186 (5)	0.4064 (2)	0.1001 (4)	0.0479 (10)	
C11	0.5191 (12)	0.7256 (4)	0.5421 (8)	0.059 (2)	0.50
H11	0.4927	0.6878	0.5423	0.071*	0.50
C12	0.604 (2)	0.8030 (6)	0.6455 (10)	0.083 (4)	0.50
H12A	0.5590	0.8252	0.5916	0.124*	0.50
H12B	0.7263	0.8063	0.6466	0.124*	0.50
H12C	0.5582	0.8159	0.7081	0.124*	0.50
C13	0.5730 (19)	0.7093 (6)	0.7196 (10)	0.087 (4)	0.50
H13A	0.4955	0.7207	0.7716	0.130*	0.50
H13B	0.6875	0.7091	0.7454	0.130*	0.50
H13C	0.5434	0.6725	0.6971	0.130*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0357 (3)	0.0334 (3)	0.0396 (4)	0.000	0.0025 (2)	0.000

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O1	0.0406 (16)	0.0403 (16)	0.0543 (19)	-0.0014 (11)	-0.0037 (12)	0.0109 (15)
O2	0.0512 (16)	0.0366 (16)	0.0608 (19)	-0.0029 (13)	-0.0145 (15)	0.0115 (14)
O3	0.0521 (16)	0.0323 (14)	0.0454 (16)	0.0016 (12)	0.0046 (13)	0.0018 (12)
O4	0.084 (3)	0.048 (2)	0.064 (2)	0.0150 (17)	0.0024 (18)	-0.0038 (18)
O5	0.076 (2)	0.058 (2)	0.048 (2)	0.0189 (17)	0.0067 (16)	-0.0077 (16)
O6	0.057 (3)	0.086 (4)	0.047 (3)	0.000	-0.008 (2)	0.000
O1W	0.071 (3)	0.082 (4)	0.058 (3)	0.000	0.010 (3)	0.000
N1	0.057 (3)	0.071 (4)	0.048 (3)	0.000	-0.006 (3)	0.000
C1	0.040 (2)	0.0340 (19)	0.037 (2)	0.0033 (16)	0.0008 (16)	-0.0024 (15)
C2	0.043 (2)	0.0330 (19)	0.051 (2)	0.0018 (17)	0.0028 (19)	0.0018 (17)
C3	0.062 (3)	0.041 (2)	0.073 (3)	0.003 (2)	0.019 (2)	0.001 (2)
C4	0.041 (2)	0.032 (2)	0.047 (2)	-0.0040 (17)	0.0019 (17)	-0.0019 (16)
C5	0.060 (3)	0.041 (2)	0.047 (2)	0.003 (2)	0.003 (2)	0.0070 (19)
C6	0.057 (2)	0.036 (2)	0.057 (3)	0.005 (2)	0.000 (2)	0.0029 (19)
C7	0.043 (2)	0.040 (2)	0.052 (3)	-0.0024 (19)	0.0035 (18)	-0.0019 (18)
C8	0.050 (2)	0.042 (2)	0.045 (2)	-0.0001 (19)	0.0000 (19)	0.0004 (18)
C9	0.051 (2)	0.034 (2)	0.050 (2)	0.0007 (18)	-0.0030 (19)	0.0026 (19)
C10	0.049 (2)	0.042 (2)	0.052 (3)	-0.0007 (19)	0.0019 (19)	-0.002 (2)
C11	0.062 (5)	0.049 (5)	0.065 (6)	-0.003 (4)	-0.001 (5)	0.002 (5)
C12	0.112 (11)	0.068 (8)	0.069 (8)	-0.021 (7)	-0.009 (8)	-0.009 (7)
C13	0.103 (10)	0.094 (10)	0.063 (7)	-0.009 (8)	-0.005 (7)	0.033 (7)

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

Sr1—O1	2.641 (3)	C2—H2	0.98
Sr1—O1 ⁱ	2.641 (3)	C3—H3A	0.96
Sr1—O2	2.712 (3)	C3—H3B	0.96
Sr1—O2 ⁱⁱ	2.549 (3)	C3—H3C	0.96
Sr1—O2 ⁱⁱⁱ	2.549 (3)	C4—C9	1.379 (6)
Sr1—O2 ⁱ	2.712 (3)	C4—C5	1.396 (6)
Sr1—O6	2.511 (5)	C5—C6	1.368 (6)
Sr1—O1W	2.688 (5)	C5—H5	0.93
O1—C1	1.257 (5)	C6—C7	1.397 (6)
O2—C1	1.257 (5)	C6—H6	0.93
O3—C4	1.373 (5)	C7—C8	1.387 (6)
O3—C2	1.431 (5)	C7—C10	1.478 (6)
O4—C10	1.218 (6)	C8—C9	1.389 (6)
O5—C10	1.319 (6)	C8—H8	0.93
O5—H5o	0.82	C9—H9	0.93
O6—C11	1.206 (11)	C11—H11	0.93
O1W—H1W	0.82	C12—H12A	0.96
N1—C12	1.327 (13)	C12—H12B	0.96
N1—C11	1.368 (11)	C12—H12C	0.96
N1—C13	1.527 (12)	C13—H13A	0.96
C1—C2	1.525 (6)	C13—H13B	0.96
C2—C3	1.521 (6)	C13—H13C	0.96
O6—Sr1—O2 ⁱⁱ	84.48 (12)	O3—C2—C3	106.3 (4)
O6—Sr1—O2 ⁱⁱⁱ	84.48 (12)	O3—C2—C1	111.6 (3)

O2 ⁱⁱ —Sr1—O2 ⁱⁱⁱ	66.84 (13)	C3—C2—C1	108.9 (3)
O6—Sr1—O1 ⁱ	92.50 (8)	O3—C2—H2	110.0
O2 ⁱⁱ —Sr1—O1 ⁱ	77.79 (10)	C3—C2—H2	110.0
O2 ⁱⁱⁱ —Sr1—O1 ⁱ	144.64 (10)	C1—C2—H2	110.0
O6—Sr1—O1	92.50 (8)	C2—C3—H3A	109.5
O2 ⁱⁱ —Sr1—O1	144.64 (10)	C2—C3—H3B	109.5
O2 ⁱⁱⁱ —Sr1—O1	77.79 (10)	H3A—C3—H3B	109.5
O1 ⁱ —Sr1—O1	137.57 (14)	C2—C3—H3C	109.5
O6—Sr1—O1W	71.44 (18)	H3A—C3—H3C	109.5
O2 ⁱⁱ —Sr1—O1W	139.05 (11)	H3B—C3—H3C	109.5
O2 ⁱⁱⁱ —Sr1—O1W	139.05 (11)	O3—C4—C9	124.7 (4)
O1 ⁱ —Sr1—O1W	70.93 (8)	O3—C4—C5	114.9 (4)
O1—Sr1—O1W	70.93 (8)	C9—C4—C5	120.3 (4)
O6—Sr1—O2	138.70 (10)	C6—C5—C4	119.6 (4)
O2 ⁱⁱ —Sr1—O2	134.19 (4)	C6—C5—H5	120.2
O2 ⁱⁱⁱ —Sr1—O2	97.29 (8)	C4—C5—H5	120.2
O1 ⁱ —Sr1—O2	107.61 (9)	C5—C6—C7	121.2 (4)
O1—Sr1—O2	48.52 (9)	C5—C6—H6	119.4
O1W—Sr1—O2	81.42 (14)	C7—C6—H6	119.4
O6—Sr1—O2 ⁱ	138.70 (10)	C8—C7—C6	118.4 (4)
O2 ⁱⁱ —Sr1—O2 ⁱ	97.29 (8)	C8—C7—C10	121.0 (4)
O2 ⁱⁱⁱ —Sr1—O2 ⁱ	134.19 (4)	C6—C7—C10	120.7 (4)
O1 ⁱ —Sr1—O2 ⁱ	48.52 (9)	C7—C8—C9	121.1 (4)
O1—Sr1—O2 ⁱ	107.61 (9)	C7—C8—H8	119.4
O1W—Sr1—O2 ⁱ	81.42 (14)	C9—C8—H8	119.4
O2—Sr1—O2 ⁱ	62.34 (12)	C4—C9—C8	119.4 (4)
C1—O1—Sr1	95.1 (2)	C4—C9—H9	120.3
C1—O2—Sr1 ^{iv}	150.8 (3)	C8—C9—H9	120.3
C1—O2—Sr1	91.8 (2)	O4—C10—O5	122.3 (5)
Sr1 ^{iv} —O2—Sr1	113.24 (10)	O4—C10—C7	124.8 (5)
C4—O3—C2	117.3 (3)	O5—C10—C7	113.0 (4)
C10—O5—H5o	120.0	O6—C11—N1	124.3 (9)
C11—O6—Sr1	131.5 (5)	O6—C11—H11	117.9
Sr1—O1W—H1W	109.5	N1—C11—H11	117.9
C12—N1—C11	126.2 (9)	N1—C12—H12A	109.5
C12—N1—C13	119.4 (10)	N1—C12—H12B	109.5
C11—N1—C13	114.2 (8)	N1—C12—H12C	109.5
O2—C1—O1	122.2 (4)	N1—C13—H13A	109.5
O2—C1—C2	117.7 (4)	N1—C13—H13B	109.5
O1—C1—C2	120.1 (4)	N1—C13—H13C	109.5
O6—Sr1—O1—C1	156.3 (3)	Sr1—O1—C1—O2	16.4 (4)
O2 ⁱⁱ —Sr1—O1—C1	-119.7 (3)	Sr1—O1—C1—C2	-160.7 (3)
O2 ⁱⁱⁱ —Sr1—O1—C1	-119.9 (3)	C4—O3—C2—C3	167.1 (4)
O1 ⁱ —Sr1—O1—C1	59.8 (4)	C4—O3—C2—C1	-74.3 (4)

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O1W—Sr1—O1—C1	86.9 (3)	O2—C1—C2—O3	154.9 (4)
O2—Sr1—O1—C1	-8.5 (2)	O1—C1—C2—O3	-27.9 (5)
O2 ⁱ —Sr1—O1—C1	12.9 (3)	O2—C1—C2—C3	-88.1 (5)
O6—Sr1—O2—C1	-14.9 (3)	O1—C1—C2—C3	89.2 (5)
O2 ⁱⁱ —Sr1—O2—C1	139.7 (2)	C2—O3—C4—C9	-2.6 (6)
O2 ⁱⁱⁱ —Sr1—O2—C1	75.1 (2)	C2—O3—C4—C5	178.4 (4)
O1 ⁱ —Sr1—O2—C1	-130.4 (2)	O3—C4—C5—C6	178.6 (4)
O1—Sr1—O2—C1	8.5 (2)	C9—C4—C5—C6	-0.4 (7)
O1W—Sr1—O2—C1	-63.6 (2)	C4—C5—C6—C7	-0.1 (7)
O2 ⁱ —Sr1—O2—C1	-148.4 (2)	C5—C6—C7—C8	0.2 (7)
O6—Sr1—O2—Sr1 ^{iv}	149.72 (15)	C5—C6—C7—C10	-179.7 (4)
O2 ⁱⁱ —Sr1—O2—Sr1 ^{iv}	-55.74 (17)	C6—C7—C8—C9	0.2 (7)
O2 ⁱⁱⁱ —Sr1—O2—Sr1 ^{iv}	-120.36 (18)	C10—C7—C8—C9	-179.9 (4)
O1 ⁱ —Sr1—O2—Sr1 ^{iv}	34.21 (16)	O3—C4—C9—C8	-178.1 (4)
O1—Sr1—O2—Sr1 ^{iv}	173.1 (2)	C5—C4—C9—C8	0.8 (6)
O1W—Sr1—O2—Sr1 ^{iv}	100.98 (14)	C7—C8—C9—C4	-0.7 (7)
O2 ⁱ —Sr1—O2—Sr1 ^{iv}	16.22 (16)	C8—C7—C10—O4	176.2 (4)
O1—Sr1—O6—C11	-28.6 (7)	C6—C7—C10—O4	-3.9 (7)
O1W—Sr1—O6—C11	40.3 (7)	C8—C7—C10—O5	-4.5 (6)
O2—Sr1—O6—C11	-11.3 (8)	C6—C7—C10—O5	175.4 (4)
Sr1—O2—C1—O1	-15.9 (4)	Sr1—O6—C11—N1	-133.9 (7)
Sr1 ^{iv} —O2—C1—C2	11.3 (8)	C12—N1—C11—O6	-0.8 (16)
Sr1—O2—C1—C2	161.2 (3)	C13—N1—C11—O6	-175.2 (10)

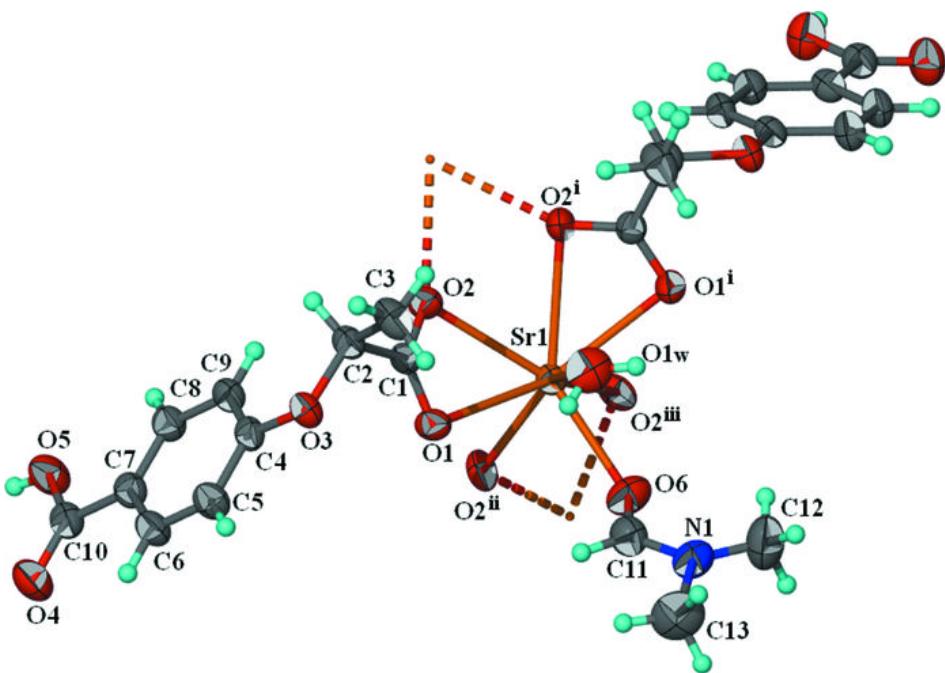
Symmetry codes: (i) $x, -y+3/2, z$; (ii) $x+1/2, -y+3/2, -z+1/2$; (iii) $x+1/2, y, -z+1/2$; (iv) $x-1/2, y, -z+1/2$.

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O5—H5O \cdots O1 ^v	0.82	1.81	2.629 (4)	174
O1W—H1W \cdots O4 ^{vi}	0.82	2.37	3.191 (5)	178

Symmetry codes: (v) $-x+1/2, -y+1, z-1/2$; (vi) $-x+1/2, y+1/2, z+1/2$.

Fig. 1



supplementary materials

Fig. 2

