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ISSN 2414-3146

Distrontium oxalate tetrahydroxidocuprate(II)

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Received 2 January 2026
Accepted 16 January 2026

Edited by M. Weil, Vienna University of Technology, Austria

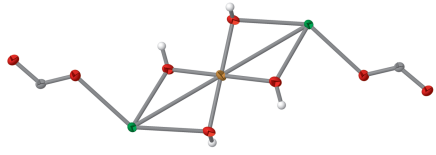
Keywords: crystal structure; inorganic; oxalate.

CCDC reference: 2523251

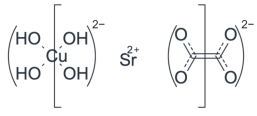
Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of distrontium oxalate tetrahydroxidocuprate(II) or poly-[tetra-μ-hydroxido-μ_6-oxalato-copperdistrontium], $Sr_2(C_2O_4)[Cu(OH)_4]$ or $[Sr_2Cu(C_2O_4)(OH)_4]_n$, has been determined in the triclinic space group $P\overline{1}$. The asymmetric unit contains one Sr, one Cu, two hydroxide groups, and half of an oxalate anion. By application of inversion symmetry, a square-planar $\{Cu(OH)_4\}$ unit and a complete oxalate anion are generated. The structure consists of a three-dimensional framework of edge-sharing $\{SrO_4(OH)_4\}$ polyhedra decorated by $\{Cu(OH)_4\}$ units and oxalate groups. Only weak hydrogen bonds are observed within the framework.

3D view



Chemical scheme



Structure description

The title compound, $Sr_2(C_2O_4)[Cu(OH)_4]$, was obtained serendipitously during attempts to synthesize $SrCu_2(BO_3)_2$ (Kageyama *et al.*, 1999) under hydrothermal conditions. Although numerous crystal structures containing Cu^{II} and oxalato ligands or oxalate anions have been reported, the combination with alkaline-earth ions is surprisingly rare. According to the Inorganic Crystal Structure Database (ICSD; version 2025–1; Zagorac *et al.*, 2019), only a few related compounds such as $Sr_2(Cu(C_2O_4)_3)(H_2O)_7$ (Insausti *et al.*, 1994) and $BaCu(C_2O_4)_2{\cdot}6H_2O$ (Hallock *et al.*, 1990; Bouayad *et al.*, 1995; Kasthuri *et al.*, 1996; Nenwa *et al.*, 2008) have been reported. Insausti and coworkers also reported the thermal analysis of $CaCu(C_2O_4)_2{\cdot}2H_2O$ and $SrCu(C_2O_4)_2{\cdot}4H_2O$, yet the crystal structures of these compounds have not been determined (Insausti *et al.*, 1993). Here, we describe the crystal structure of $Sr_2(C_2O_4)[Cu(OH)_4]$.

The crystal structure of $Sr_2(C_2O_4)[Cu(OH)_4]$ consists of a three-dimensional framework built from Sr^{II} cations coordinated by $\{Cu(OH)_4\}^{2-}$ and oxalate $(C_2O_4)^{2-}$ units (Figs. 1 and 2). The asymmetric unit comprises one Sr^{II}, one Cu^{II}, two (OH) groups, and half of an oxalate anion. By application of inversion symmetry, a $\{Cu(OH)_4\}$ square-planar unit and the full oxalate anion are generated. The coordination environment around Sr is an $\{SrO_4(OH)_4\}$ polyhedron, which resembles a square antiprism but is significantly distorted in the triclinic lattice. Each oxalate anion bonds to six Sr^{II} cations, with four

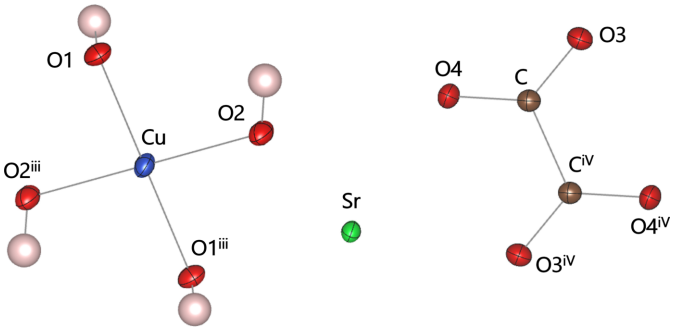


Figure 1
The asymmetric unit of the title compound expanded to visualize the complete $\{Cu(OH)_4\}^{2-}$ unit and the oxalate anion. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (iii) $-x+1, -y, -z+1$, (iv) $-x, -y+1, -z+2$.]

bridging and two chelating modes. The $\{Cu(OH)_4\}$ units are oriented nearly perpendicular to the crystallographic [111] direction (Fig. 3). The OH^- groups of the $\{Cu(OH)_4\}$ unit do not form obvious hydrogen bonds with the surrounding oxygen atoms of the oxalate anions. The O1···O4′ and O2···O3′ distances are around 3.0 Å, however, the O—H···O angles are strongly bent from 180° (104 and 121°, respectively), indicating that these hydrogen bonds are rather weak.

Synthesis and crystallization

$Sr(OH)_2{\cdot}8H_2O$ (1.4 g), $Cu(OH)_2$ (0.1 g), acetylacetone ($C_5H_8O_2$, 0.2 ml), H_3BO_3 (0.03 g), and distilled water (10 ml) were placed in a Teflon-lined stainless-steel autoclave and heated at 473 K for 24 h. All reagents were purchased from FUJIFILM Wako and used without further purification. The oxalate ions are likely generated through the oxidative decomposition of acetylacetone under the alkaline reaction conditions. Violet, rhombic plates were obtained, and a single crystal was selected for X-ray diffraction at room temperature.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Sr_2Cu(C_2O_4)(OH)_4]$
M_r	394.84
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	6.0754 (3), 6.5442 (3), 6.5466 (2)
α, β, γ (°)	103.712 (3), 117.235 (4), 106.601 (4)
V (Å^3)	200.06 (2)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	20.54
Crystal size (mm)	0.08 × 0.06 × 0.01
Data collection	
Diffractometer	XtaLAB Synergy R, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.705, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1612, 785, 774
R_{int}	0.019
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.049, 1.07
No. of reflections	785
No. of parameters	64
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.48

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *VESTA 3* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 1. H atoms were located from difference syntheses and were refined using a riding model (AFIX 147 instruction; Sheldrick, 2015*b*).

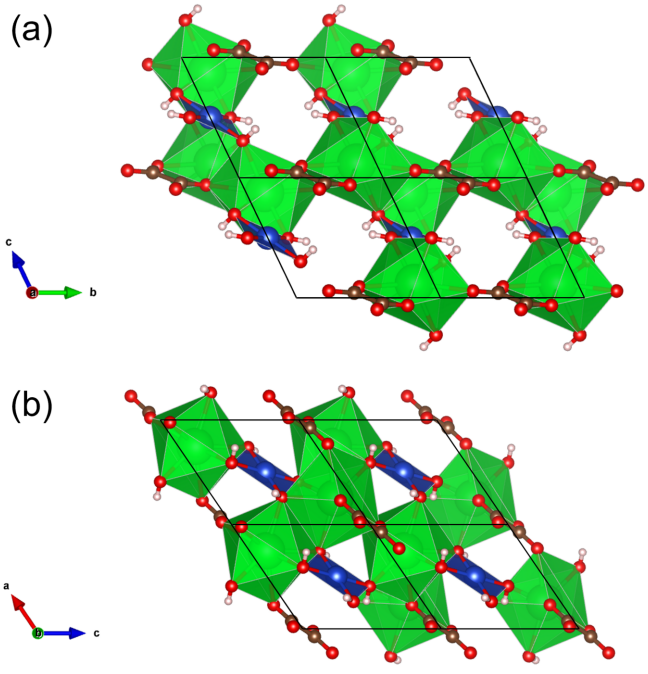


Figure 2
Three-dimensional framework of the crystal structure with polyhedral representation of the $\{SrO_4(OH)_4\}$ (green) and $\{Cu(OH)_4\}$ (blue) building units, as viewed along the (*a*) *a* and (*b*) *b* axes.

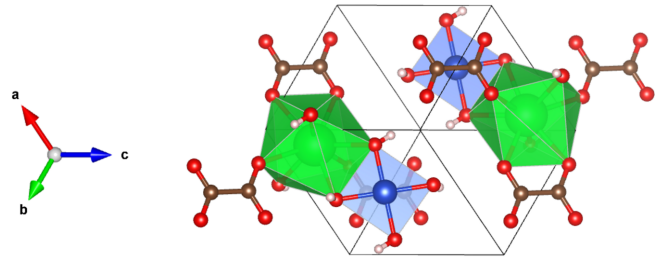


Figure 3
The expanded unit cell of the title compound viewed along the [111] direction; color codes are as in Fig. 2.

Acknowledgements

The XRD experiment was performed as joint research at the Institute for Solid State Physics, UTokyo (Project No. 202410-MCBXG-0002) and using the Rigaku XtaLAB Synergy-*R* at the Molecular Structure Analysis Section, Shizuoka Instrumental Analysis Center, Shizuoka University.

Funding information

Funding for this research was provided by: Japan Society for the Promotion of Science.

References

Bouayad, A., Trombe, J.-C. & Gleizes, A. (1995). *Inorg. Chim. Acta* **230**, 1–7.
Hallock, R. B., Rhine, W. E., Cima, M. J., Bott, S. & Atwood, J. (1990). *Ceram. Trans.* **13**, 251–258.
Insausti, M., Cortes, R., Rojo, T., Bocanegra, E. H. & Arriortua, M. (1993). *Solid State Ionics* **63–65**, 351–357.
Insausti, M., Urtiaga, M. K., Cortés, R., Mesa, J. L., Arriortua, M. I. & Rojo, T. (1994). *J. Mater. Chem.* **4**, 1867–1870.
Kageyama, H., Onizuka, K., Yamauchi, T. & Ueda, Y. (1999). *J. Cryst. Growth* **206**, 65–67.
Kasthuri, V. B., Rao, P. M. & Nethaji, M. (1996). *Cryst. Res. Technol.* **31**, 287–294.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Nenwa, J., Belombe, M. M., Fokwa, B. P. T. & Dronskowski, R. (2008). *Acta Cryst.* E**64**, m116–m117.
Rigaku OD (2023). *CrysAlis PRO*. Rigaku Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zagorac, D., Müller, H., Ruehl, S., Zagorac, J. & Rehme, S. (2019). *J. Appl. Cryst.* **52**, 918–925.

full crystallographic data

IUCrData (2026). **11**, x260043 [https://doi.org/10.1107/S241431462600043X]

Distrontium oxalate tetrahydroxidocuprate(II)

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Poly[tetra-μ-hydroxido-μ_6-oxalato-copperdistrontium]

Crystal data

$[CuSr_2(C_2O_4)(OH)_4]$
M_r = 394.84
Triclinic, $P\overline{1}$
a = 6.0754 (3) Å
b = 6.5442 (3) Å
c = 6.5466 (2) Å
α = 103.712 (3)°
β = 117.235 (4)°
γ = 106.601 (4)°
V = 200.06 (2) Å^3
Z = 1
$F(000)$ = 185
D_x = 3.277 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1429 reflections
θ = 7.8–75.7°
μ = 20.54 mm^{-1}
T = 293 K
Plate, translucent, violet
0.08 × 0.06 × 0.01 mm

Data collection

XtaLAB Synergy R, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2023)
T_{min} = 0.705, T_{max} = 1.000
1612 measured reflections
785 independent reflections
774 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 76.6°, θ_{min} = 7.8°
h = −7→7
k = −4→8
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.049
S = 1.07
785 reflections
64 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 0.1268P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: SHELXL2019/2 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0151 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Hydrogen atoms were located from difference syntheses. All O—H hydrogen atoms were refined using the AFIX 147 riding model (Sheldrick, 2015*b*).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr	0.25216 (5)	0.13033 (4)	0.87805 (4)	0.01415 (14)
Cu	0.500000	0.000000	0.500000	0.01451 (17)
C	0.0730 (5)	0.5793 (4)	0.9551 (5)	0.0137 (5)
O1	0.5900 (4)	0.1511 (4)	0.3047 (4)	0.0187 (4)
O2	0.2604 (4)	0.1402 (4)	0.4994 (4)	0.0194 (4)
O3	0.0218 (5)	0.7498 (4)	0.9402 (4)	0.0228 (4)
O4	0.2296 (5)	0.5243 (4)	0.9062 (5)	0.0234 (5)
H1	0.733912	0.275791	0.402865	0.028*
H2	0.299239	0.256363	0.471123	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr	0.01757 (18)	0.01766 (18)	0.01888 (19)	0.01191 (12)	0.01421 (14)	0.01195 (13)
Cu	0.0152 (3)	0.0194 (3)	0.0155 (3)	0.0094 (2)	0.0114 (3)	0.0095 (2)
C	0.0144 (12)	0.0129 (12)	0.0151 (13)	0.0064 (10)	0.0088 (11)	0.0070 (10)
O1	0.0232 (10)	0.0207 (10)	0.0206 (10)	0.0102 (8)	0.0162 (9)	0.0128 (8)
O2	0.0220 (10)	0.0264 (11)	0.0246 (11)	0.0154 (9)	0.0175 (9)	0.0181 (9)
O3	0.0315 (11)	0.0201 (10)	0.0370 (12)	0.0174 (9)	0.0268 (10)	0.0193 (9)
O4	0.0291 (11)	0.0220 (10)	0.0416 (13)	0.0169 (9)	0.0297 (11)	0.0197 (10)

Geometric parameters (Å, º)

Sr—O2	2.518 (2)	Sr—Sr^{ii}	3.9910 (5)
Sr—O1^{i}	2.539 (2)	Cu—O2^{iii}	1.9287 (18)
Sr—O2^{ii}	2.583 (2)	Cu—O2	1.9287 (18)
Sr—O4	2.588 (2)	Cu—O1^{iii}	1.9603 (19)
Sr—O1^{iii}	2.600 (2)	Cu—O1	1.9603 (19)
Sr—O3^{iv}	2.630 (2)	C—O4	1.248 (3)
Sr—O3^{v}	2.708 (2)	C—O3	1.254 (3)
Sr—O4^{vi}	2.714 (2)	C—C^{iv}	1.565 (5)
Sr—Cu	3.5020 (2)	O1—H1	0.8200
Sr—Cu^{vii}	3.7623 (3)	O2—H2	0.8200
Sr—Sr^{viii}	3.7886 (4)		
O2—Sr—O1^{i}	135.38 (6)	O4—Sr—Sr^{ii}	88.07 (5)
O2—Sr—O2^{ii}	77.03 (7)	O1^{iii}—Sr—Sr^{ii}	74.17 (5)
O1^{i}—Sr—O2^{ii}	137.35 (6)	O3^{iv}—Sr—Sr^{ii}	106.34 (5)
O2—Sr—O4	80.99 (6)	O3^{v}—Sr—Sr^{ii}	99.03 (5)
O1^{i}—Sr—O4	113.62 (7)	O4^{vi}—Sr—Sr^{ii}	115.39 (5)
O2^{ii}—Sr—O4	95.78 (7)	Cu—Sr—Sr^{ii}	59.857 (6)
O2—Sr—O1^{iii}	63.16 (6)	Cu^{vii}—Sr—Sr^{ii}	53.604 (6)

O1^{i}—Sr—O1^{iii}	85.00 (7)	Sr^{viii}—Sr—Sr^{ii}	115.634 (11)
O2^{ii}—Sr—O1^{iii}	91.06 (6)	O2^{iii}—Cu—O2	180.0
O4—Sr—O1^{iii}	140.92 (6)	O2^{iii}—Cu—O1^{iii}	92.84 (8)
O2—Sr—O3^{iv}	132.05 (6)	O2—Cu—O1^{iii}	87.16 (8)
O1^{i}—Sr—O3^{iv}	89.39 (7)	O2^{iii}—Cu—O1	87.16 (8)
O2^{ii}—Sr—O3^{iv}	77.40 (7)	O2—Cu—O1	92.84 (8)
O4—Sr—O3^{iv}	62.15 (6)	O1^{iii}—Cu—O1	180.00 (6)
O1^{iii}—Sr—O3^{iv}	156.01 (6)	O2^{iii}—Cu—Sr	135.56 (6)
O2—Sr—O3^{v}	128.48 (7)	O2—Cu—Sr	44.44 (6)
O1^{i}—Sr—O3^{v}	68.85 (7)	O1^{iii}—Cu—Sr	47.09 (6)
O2^{ii}—Sr—O3^{v}	68.65 (7)	O1—Cu—Sr	132.91 (6)
O4—Sr—O3^{v}	138.09 (6)	O2^{iii}—Cu—Sr^{iii}	44.44 (6)
O1^{iii}—Sr—O3^{v}	79.93 (6)	O2—Cu—Sr^{iii}	135.56 (6)
O3^{iv}—Sr—O3^{v}	76.30 (7)	O1^{iii}—Cu—Sr^{iii}	132.91 (6)
O2—Sr—O4^{vi}	76.83 (7)	O1—Cu—Sr^{iii}	47.09 (6)
O1^{i}—Sr—O4^{vi}	69.84 (7)	Sr—Cu—Sr^{iii}	180.0
O2^{ii}—Sr—O4^{vi}	152.23 (6)	O2^{iii}—Cu—Sr^{ii}	140.54 (6)
O4—Sr—O4^{vi}	71.00 (7)	O2—Cu—Sr^{ii}	39.46 (6)
O1^{iii}—Sr—O4^{vi}	85.41 (6)	O1^{iii}—Cu—Sr^{ii}	86.22 (6)
O3^{iv}—Sr—O4^{vi}	114.46 (7)	O1—Cu—Sr^{ii}	93.78 (6)
O3^{v}—Sr—O4^{vi}	137.07 (7)	Sr—Cu—Sr^{ii}	66.539 (7)
O2—Sr—Cu	32.44 (4)	Sr^{iii}—Cu—Sr^{ii}	113.461 (8)
O1^{i}—Sr—Cu	106.01 (4)	O2^{iii}—Cu—Sr^{ix}	39.46 (6)
O2^{ii}—Sr—Cu	92.68 (4)	O2—Cu—Sr^{ix}	140.54 (6)
O4—Sr—Cu	107.57 (5)	O1^{iii}—Cu—Sr^{ix}	93.78 (6)
O1^{iii}—Sr—Cu	33.52 (4)	O1—Cu—Sr^{ix}	86.22 (6)
O3^{iv}—Sr—Cu	164.31 (5)	Sr—Cu—Sr^{ix}	113.461 (7)
O3^{v}—Sr—Cu	111.68 (4)	Sr^{iii}—Cu—Sr^{ix}	66.539 (8)
O4^{vi}—Sr—Cu	69.58 (5)	Sr^{ii}—Cu—Sr^{ix}	180.0
O2—Sr—Cu^{vii}	87.84 (5)	O4—C—O3	126.4 (2)
O1^{i}—Sr—Cu^{vii}	136.43 (5)	O4—C—C^{iv}	116.8 (3)
O2^{ii}—Sr—Cu^{vii}	28.33 (4)	O3—C—C^{iv}	116.8 (3)
O4—Sr—Cu^{vii}	71.54 (5)	Cu—O1—Sr^{x}	127.46 (10)
O1^{iii}—Sr—Cu^{vii}	119.12 (5)	Cu—O1—Sr^{iii}	99.39 (8)
O3^{iv}—Sr—Cu^{vii}	53.30 (5)	Sr^{x}—O1—Sr^{iii}	95.00 (7)
O3^{v}—Sr—Cu^{vii}	79.79 (5)	Cu—O1—H1	109.5
O4^{vi}—Sr—Cu^{vii}	141.23 (4)	Sr^{x}—O1—H1	115.8
Cu—Sr—Cu^{vii}	113.461 (7)	Sr^{iii}—O1—H1	103.2
O2—Sr—Sr^{viii}	99.63 (4)	Cu—O2—Sr	103.13 (8)
O1^{i}—Sr—Sr^{viii}	43.12 (4)	Cu—O2—Sr^{ii}	112.21 (9)
O2^{ii}—Sr—Sr^{viii}	120.37 (4)	Sr—O2—Sr^{ii}	102.97 (7)
O4—Sr—Sr^{viii}	143.24 (5)	Cu—O2—H2	109.5
O1^{iii}—Sr—Sr^{viii}	41.88 (5)	Sr—O2—H2	126.4
O3^{iv}—Sr—Sr^{viii}	128.30 (5)	Sr^{ii}—O2—H2	102.5
O3^{v}—Sr—Sr^{viii}	68.79 (5)	C—O3—Sr^{iv}	120.51 (17)
O4^{vi}—Sr—Sr^{viii}	73.39 (4)	C—O3—Sr^{xi}	133.28 (17)
Cu—Sr—Sr^{viii}	67.216 (6)	Sr^{iv}—O3—Sr^{xi}	103.70 (7)
Cu^{vii}—Sr—Sr^{viii}	145.022 (10)	C—O4—Sr	122.20 (17)

O2—Sr—Sr^{ii}	39.09 (5)	C—O4—Sr^{vi}	117.75 (17)
O1^{i}—Sr—Sr^{ii}	157.66 (5)	Sr—O4—Sr^{vi}	109.00 (7)
O2^{ii}—Sr—Sr^{ii}	37.93 (4)		
O4—C—O3—Sr^{iv}	−170.3 (2)	O3—C—O4—Sr	−170.1 (2)
C^{iv}—C—O3—Sr^{iv}	9.5 (4)	C^{iv}—C—O4—Sr	10.2 (4)
O4—C—O3—Sr^{xi}	−11.5 (5)	O3—C—O4—Sr^{vi}	49.9 (4)
C^{iv}—C—O3—Sr^{xi}	168.3 (2)	C^{iv}—C—O4—Sr^{vi}	−129.9 (3)

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, −*y*+1, −*z*+2; (vii) *x*−1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*+2; (ix) *x*+1, *y*, *z*; (x) *x*, *y*, *z*−1; (xi) *x*, *y*+1, *z*.