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$Sr_9La_2(WO_6)_4$ containing $[WO_6]$ octahedra

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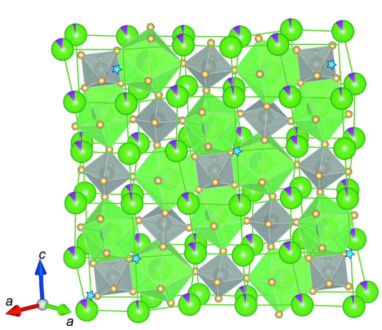
A polycrystalline sample of $Sr_9La_2(WO_6)_4$, nonastrontium dilanthanum tetrakis[orthotungstate(VI)], was prepared by heating a compacted powder mixture of $SrCO_3$, WO_3, and La_2O_3 with an Sr:La:W molar ratio of 9:2:4 at 1473 K. X-ray crystal structure analysis was performed for a $Sr_9La_2(WO_6)_4$ single-crystal grain grown by reheating the sample at 1673 K. $Sr_9La_2(WO_6)_4$ crystallizes with four formula units in the tetragonal space group $I4_1/a$ and is isotypic with $Sr_{11}(ReO_6)_4$. Two W sites with site symmetries of $\overline{1}$ are located at the center of isolated $[WO_6]$ octahedra, and four mixed (Sr/La) sites are surrounded by eight to twelve O atoms of the $[WO_6]$ octahedra. The structure of $Sr_9La_2(WO_6)_4$ can be described on the basis of the double-perovskite structure with $[WO_6]$ and $[(Sr/La)O_x]$ polyhedra alternately placed, and a vacancy (□).

1. Chemical context

The alkaline-earth (A) rare-earth (Ln) tungstates $A_9Ln_2(WO_6)_4$ have attracted attention as host crystals of phosphors, and various luminescence properties of these tungstates doped with activators such as Eu^{3+} and Mn^{4+} have been evaluated. For example, emissions of Eu^{3+} at ~615 nm excited by ~395 nm wavelength light have been reported for $Sr_9Gd_{1.5}Eu_{0.5}(WO_6)_4$ (Blasse & Kemmler-Sack, 1983), $Ca_9Gd_{2-x}Eu_x(WO_6)_4$ (Zeng *et al.*, 2013), $Ca_9Eu_2(WO_6)_4$ (Qin *et al.*, 2012; Zeng *et al.*, 2010), $Sr_9Eu_2(WO_6)_4$ (Qin *et al.*, 2012; Blasse & Kemmler-Sack, 1983; Zeng *et al.*, 2010), and $Ca_{9-x}Sr_xEu_2(WO_6)_4$ (Zeng *et al.*, 2009). Mn^{4+}-doped $Sr_9Y_2(WO_6)_4$ (Shi *et al.*, 2019) and Mn^{4+}/Mg^{2+}-doped $Sr_9Y_2(WO_6)_4$ (Zhou *et al.*, 2020) were also studied, and deep-red luminescence with broad emission maxima at ~680 nm were observed under excitation by light with a wavelength of 365 nm.

Unit-cell parameters of a tetragonal cell with a = 11.664 (2) Å, c = 16.335 (4) Å (Smirnov *et al.*, 1987) and a = 16.44 (7) Å, c = 16.32 (3) Å (Kemmler-Sack & Ehmann, 1981) have been reported for $Sr_9La_2(WO_6)_4$. However, details of the crystal structure, including atom positions, have not been clarified up to now. $Sr_9Ln_2(WO_6)_4$ compounds prepared by substituting Ln (a rare-earth element) for La in $Sr_9La_2(WO_6)_4$ have also been reported. These materials have tetragonal symmetry for Ln = La, Pr, and Nd; cubic (high-temperature phase) and tetragonal (low-temperature phase) symmetry for Sm, Eu, and Gd; monoclinic symmetry for Tb and Dy; and cubic symmetry for Ho, Er, Tm, and Y (Kemmler-Sack & Ehmann, 1981). The Sr atoms of $Sr_9La_2(WO_6)_4$ can also be replaced with Ca or Ba. For $Ca_9Ln_2(WO_6)_4$ (Ln = Nd, Sm, Eu, Gd, Tb, Dy), lattice parameters of a tetragonal unit-cell with $11.05 \le a \le 11.13$ Å and $16.37 \le c \le 16.42$ Å and space group



$I4_1/a$ have been reported (Smirnov *et al.*, 1987). $Ba_9Ln_2(WO_6)_4$ compounds (Ln = La, Nd, Sm, Eu) are cubic ($8.50 \leq a \leq 8.56$ Å; Betz *et al.*, 1982). The crystal structures of $Sr_9Gd_2(WO_6)_4$ [$Fm\overline{3}$, a = 16.47013 (6) Å] and $Ba_9La_2(WO_6)_4$ [$Fm\overline{3}$, a = 17.12339 (15) Å] have been fully analyzed (Ijdo *et al.*, 2016). However, atomic positions for the tetragonal structures of $Ca_9Ln_2(WO_6)_4$ (Ln = Nd, Sm, Eu, Gd, Tb, Dy) compounds have not been determined.

Here, we report on synthesis and crystal structure analysis of $Sr_9La_2(WO_6)_4$.

2. Structural commentary

The unit-cell parameters of $Sr_9La_2(WO_6)_4$ determined in the present investigation are consistent with those reported in previous studies (Smirnov *et al.*, 1987; Kemmler-Sack & Ehmann, 1981). Fig. 1 displays the principal building units in the crystal structure of $Sr_9La_2(WO_6)_4$. W1 (multiplicity and Wyckoff letter 8d with site symmetry $\overline{1}$) and W2 (8c, $\overline{1}$) each are located at the center of a [WO_6] octahedron. The [WO_6] octahedra are isolated and surrounded by mixed-occupied (Sr,La) atoms. As detailed in Table 1, the interatomic distances between W and O are 1.901 (4)–1.934 (4) Å (average: 1.922 Å) for W1—O and 1.891 (4)–1.967 (4) Å (average: 1.925 Å) for W2—O. The bond-valence sums (BVS; Brown & Altermatt, 1985) for W1 and W2, as calculated using the parameters for W—O (R_0 = 1.921, B = 0.37) (Brese & O'Keeffe, 1991), are 5.994 and 5.957 valence units, respectively. These values are consistent with the valence state +VI for W.

The Sr/La occupancies for (Sr/La)1 (16f, 1), (Sr/La)2 (16f, 1), (Sr/La)3 (8e, 2..), and (Sr/La)4 (4a, $\overline{4}$..) are 0.6384/0.3616 (19), 0.8913/0.1087 (18), 0.948/0.052 (4), and 0.985/0.015 (7), respectively. The interatomic distances between (Sr/La) and O and the coordination numbers of the cations are 2.333 (4)–2.861 (4) Å (average: 2.611 Å) and 8 for (Sr/La)1—O; 2.470 (4)–2.877 (5) Å (average: 2.660 Å) and 8 for (Sr/La)2—O; 2.557 (4)–3.220 (4) Å (average: 2.761 Å) and 10 for (Sr/La)3—O; and 2.607 (4)–3.131 (4) Å (average: 2.912 Å) and 12 for (Sr/La)4—O. As the La occupancy increases, the (Sr/La)—O interatomic distance decreases.

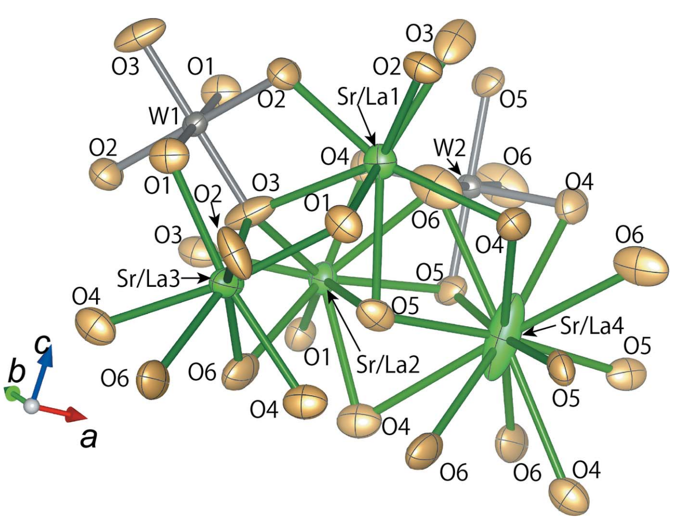


Figure 1
The principal building units in the crystal structure of $Sr_9La_2(WO_6)_4$ with displacement ellipsoids drawn at the 99% probability level. Symmetry codes refer to Table 1.

Table 1
Selected bond lengths (Å).

Sr1/La1—O6^{i}	2.333 (4)	Sr3/La3—O1^{x}	3.220 (4)
Sr1/La1—O2	2.438 (4)	Sr4/La4—O1	2.607 (4)
Sr1/La1—O2^{ii}	2.453 (4)	Sr4/La4—O1^{vi}	2.607 (4)
Sr1/La1—O4^{iii}	2.458 (4)	Sr4/La4—O1^{xi}	2.607 (4)
Sr1/La1—O5^{iv}	2.728 (4)	Sr4/La4—O1^{ix}	2.607 (4)
Sr1/La1—O3^{iii}	2.765 (5)	Sr4/La4—O4	2.998 (5)
Sr1/La1—O3	2.849 (5)	Sr4/La4—O4^{xi}	2.998 (5)
Sr1/La1—O1^{iii}	2.861 (4)	Sr4/La4—O4^{ix}	2.998 (5)
Sr2/La2—O3^{v}	2.470 (4)	Sr4/La4—O4^{vi}	2.998 (5)
Sr2/La2—O1^{vi}	2.548 (4)	Sr4/La4—O5^{i}	3.131 (4)
Sr2/La2—O6	2.599 (4)	Sr4/La4—O5^{xii}	3.131 (4)
Sr2/La2—O2^{vii}	2.603 (4)	Sr4/La4—O5^{v}	3.131 (4)
Sr2/La2—O1	2.642 (4)	Sr4/La4—O5^{viii}	3.131 (4)
Sr2/La2—O5	2.652 (4)	W1—O3	1.901 (4)
Sr2/La2—O5^{v}	2.704 (4)	W1—O3^{xiii}	1.901 (4)
Sr2/La2—O4	2.777 (4)	W1—O6^{viii}	1.930 (4)
Sr2/La2—O4^{v}	2.877 (5)	W1—O6^{xiv}	1.930 (4)
Sr3/La3—O6^{i}	2.557 (4)	W1—O2	1.934 (4)
Sr3/La3—O6^{viii}	2.557 (4)	W1—O2^{xiii}	1.934 (4)
Sr3/La3—O5^{viii}	2.596 (4)	W2—O4^{xi}	1.891 (4)
Sr3/La3—O5^{i}	2.596 (4)	W2—O4^{v}	1.891 (4)
Sr3/La3—O3	2.660 (4)	W2—O1^{xv}	1.917 (4)
Sr3/La3—O3^{ix}	2.660 (4)	W2—O1	1.917 (4)
Sr3/La3—O4^{ix}	2.773 (4)	W2—O5^{xi}	1.967 (4)
Sr3/La3—O4	2.773 (4)	W2—O5^{v}	1.967 (4)
Sr3/La3—O1^{iii}	3.220 (4)		

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-y+\frac{1}{4}, x+\frac{1}{4}, -z+\frac{5}{4}$; (iii) $y+\frac{1}{4}, -x+\frac{1}{4}, z+\frac{1}{4}$; (iv) $y+\frac{1}{4}, -x+\frac{3}{4}, -z+\frac{3}{4}$; (v) $-y+\frac{1}{4}, x-\frac{1}{4}, z-\frac{1}{4}$; (vi) $-y+\frac{1}{4}, x+\frac{1}{4}, -z+\frac{1}{4}$; (vii) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$; (viii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (ix) $-x, -y+\frac{1}{2}, z$; (x) $-y-\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$; (xi) $y-\frac{1}{4}, -x+\frac{1}{4}, -z+\frac{1}{4}$; (xii) $y-\frac{1}{4}, -x+\frac{3}{4}, z-\frac{1}{4}$; (xiii) $-x, -y, -z+1$; (xiv) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$; (xv) $-x, -y, -z$.

The crystal structures of alkaline-earth and rare-earth tungstates are often described in relation to the double-perovskite structure type (Kemmler-Sack & Ehmann, 1981; Betz *et al.*, 1982; Blasse & Kemmler-Sack, 1983; King *et al.*, 2010; Ijdo *et al.*, 2016). In the double-perovskite ($A_2BB'O_6$) structure, B and B' atoms alternately occupy the B site of the perovskite (ABO_3) structure. The B site is at the center of an octahedron formed by O atoms, and the vertex-sharing [BO_6] and [$B'O_6$] octahedra regularly align in the A_8 simple cubic lattice frame in the double-perovskite structure. In case of the structure of $Sr_9La_2(WO_6)_4$, a (Sr/La,□)$_8$ distorted simple lattice can be derived by connecting the Sr-rich sites of (Sr/La)2, (Sr/La)3, and (Sr/La)4 and a vacancy site at (1/2, 3/4, 1/8), as shown in Fig. 2. In the distorted lattice, the [WO_6] octahedra and the [(Sr/La)1O_8] polyhedra are alternately located by sharing four vertices and two edges of the [(Sr/La)1O_8] polyhedra (Fig. 2).

The crystal structure of $Sr_9La_2(WO_6)_4$ is isotypic with those of $Sr_{11}(ReO_6)_4$ [a = 11.6779 (1), c = 16.1488 (2); Bramnik *et al.*, 2000], $Ba_{11}(OsO_6)_4$ [a = 12.2414 (1), c = 16.6685 (1); Wakeshima & Hinatsu, 2005], $La_9Sr(IrO_6)_4$ [a = 11.5955 (11), c = 16.2531 (15); Ferreira *et al.*, 2018], and $Sr_{11}(MoO_6)_4$ [a = 11.6107 (6), c = 16.4219 (13); Löpez *et al.*, 2016].

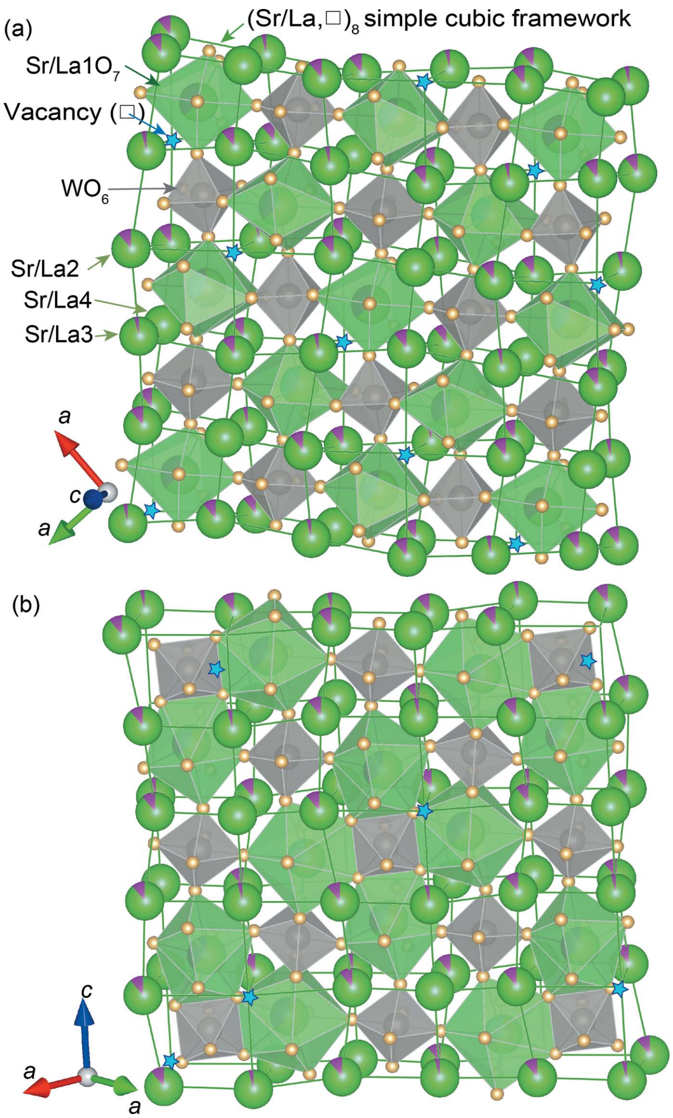


Figure 2
$[WO_6]$ octahedra and $[(Sr/La)1O_8]$ polyhedra alternately distributed in the distorted $(Sr/La2–4,\square)_8$ lattice as illustrated for the planes parallel to (001) in (*a*) and (110) in (*b*). Note that $[WO_6]$ octahedra and $[(Sr/La)1O_8]$ polyhedra are connected to each other by vertex- or edge-sharing.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Sr_9La_2(WO_6)_4$
M_r	2185.80
Crystal system, space group	Tetragonal, $I4_1/a$
Temperature (K)	300
a, c (Å)	11.6365 (3), 16.3040 (4)
V (Å^3)	2207.69 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	46.16
Crystal size (mm)	0.05 × 0.04 × 0.03
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.20, 0.33
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	62981, 2106, 1972
R_{int}	0.048
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.046, 1.37
No. of reflections	2106
No. of parameters	97
No. of restraints	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.14, −1.50

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

3. Synthesis and crystallization

Raw powdered materials of $SrCO_3$ (Hakushin Chemical Laboratory, 98%), WO_3 (Furuuchi Chemical, 99.99%), and La_2O_3 (FUJIFILM Wako Pure Chemical, 99.99%; calcined at 1273 K in advance) were weighed in a Sr:La:W molar ratio of 9:2:4, mixed in an agate mortar, and pressed into a cylindrical pellet with a diameter of 6 mm. The pellet was placed on a Pt plate in an alumina crucible with a lid (Nikkato, SSA-S) and heated to 1473 K at a rate of 300 K h^{-1} in a furnace. This temperature was maintained for 10 h, and the power to the heater of the furnace was then shut off. After the sample had cooled to room temperature, the sintered pellet was crushed, pressed into a pellet, and heated again under the same conditions. This procedure was performed three times. Part of the sintered pellet was then placed on a Pt plate in an alumina crucible, heated at 1673 K for 6 h, and cooled to room temperature at a rate of −400 K h^{-1}. The obtained crystalline sample was an aggregate consisting of ~50 µm single-crystalline grains. A single crystal selected from the aggregate was placed on top of a glass fiber for X-ray structure analysis. Another single crystal was embedded in resin, mirror polished, and carbon coated in preparation for chemical analysis using an electron microprobe analyzer (EPMA; JEOL JXA-8200). The chemical composition determined by EPMA was Sr: 23.2 (4), La: 4.8 (1), W: 10.3 (3), and O: 61.7 (5) wt%. The Sr:La:W:O atomic ratio of 9.1 (1): 1.9 (1): 4.0 (1): 24.0 (2) calculated from the composition is consistent with the chemical formula $Sr_9La_2(WO_6)_4$.

4. Refinement

The results of the crystal structure analysis are summarized in Table 2. An initial structure model with two W sites, four Sr sites, and six O sites using isotropic displacement parameters showed residual electron density distribution around the four Sr sites. These sites were changed to Sr/La mixed sites, and their occupancies were refined under consideration of full occupancy, resulting in an Sr:La:W:O atomic ratio of 35.6:8.4:16:96. Given the charge balance, the numbers of Sr and La atoms in the unit cell was constrained to be 36 and 8, respectively.

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supporting information

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$Sr_9La_2(WO_6)_4$ containing [WO_6] octahedra

Rayko Simura, Tomoki Watanabe and Hisanori Yamane

Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Nonastrontium dilanthanum tetrakis[orthotungstate(VI)]

Crystal data

$Sr_9La_2(WO_6)_4$
M_r = 2185.80
Tetragonal, $I4_1/a$
a = 11.6365 (3) Å
c = 16.3040 (4) Å
V = 2207.69 (13) Å^3
Z = 4
F(000) = 3776
D_x = 6.576 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9792 reflections
θ = 3.5–33.2°
μ = 46.16 mm^{-1}
T = 300 K
Granular, translucent colourless
0.05 × 0.04 × 0.03 mm

Data collection

Bruker D8 QUEST diffractometer
Radiation source: sealed X-ray tube
Detector resolution: 7.3910 pixels mm^{-1}
ω and σcans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.20, T_{max} = 0.33
62981 measured reflections
2106 independent reflections
1972 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 33.2°, θ_{min} = 2.2°
h = −17→17
k = −17→17
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.046
S = 1.37
2106 reflections
97 parameters
1 restraint
$w = 1/[\sigma^2(F_o^2) + 62.4087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −1.50 e Å^{-3}
Extinction correction: SHELXL-2014/7 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000055 (5)

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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.20878 (3)	0.22538 (3)	0.53417 (2)	0.00769 (8)	0.6384 (19)
La1	0.20878 (3)	0.22538 (3)	0.53417 (2)	0.00769 (8)	0.3616 (19)
Sr2	0.23647 (4)	0.04341 (4)	0.11357 (3)	0.00718 (9)	0.8913 (18)
La2	0.23647 (4)	0.04341 (4)	0.11357 (3)	0.00718 (9)	0.1087 (18)
Sr3	0.0000	0.2500	0.36535 (4)	0.00934 (14)	0.948 (4)
La3	0.0000	0.2500	0.36535 (4)	0.00934 (14)	0.052 (4)
Sr4	0.0000	0.2500	0.1250	0.0267 (4)	0.985 (7)
La4	0.0000	0.2500	0.1250	0.0267 (4)	0.015 (7)
W1	0.0000	0.0000	0.5000	0.00522 (6)	
W2	0.0000	0.0000	0.0000	0.00502 (6)	
O1	0.0101 (3)	0.0266 (3)	0.1158 (2)	0.0093 (7)	
O2	0.0795 (3)	0.0786 (3)	0.5877 (2)	0.0099 (7)	
O3	0.1059 (4)	0.0651 (4)	0.4243 (3)	0.0137 (8)	
O4	0.1383 (4)	0.1321 (4)	0.2554 (3)	0.0148 (8)	
O5	0.3675 (3)	0.1315 (3)	0.2308 (2)	0.0109 (7)	
O6	0.4011 (3)	0.1285 (3)	0.0246 (2)	0.0096 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.00728 (15)	0.00640 (15)	0.00939 (16)	0.00166 (12)	−0.00049 (12)	0.00060 (12)
La1	0.00728 (15)	0.00640 (15)	0.00939 (16)	0.00166 (12)	−0.00049 (12)	0.00060 (12)
Sr2	0.00722 (17)	0.00602 (17)	0.00830 (18)	−0.00036 (14)	0.00015 (14)	−0.00025 (14)
La2	0.00722 (17)	0.00602 (17)	0.00830 (18)	−0.00036 (14)	0.00015 (14)	−0.00025 (14)
Sr3	0.0127 (3)	0.0080 (3)	0.0074 (3)	−0.0024 (2)	0.000	0.000
La3	0.0127 (3)	0.0080 (3)	0.0074 (3)	−0.0024 (2)	0.000	0.000
Sr4	0.0091 (3)	0.0091 (3)	0.0620 (10)	0.000	0.000	0.000
La4	0.0091 (3)	0.0091 (3)	0.0620 (10)	0.000	0.000	0.000
W1	0.00463 (11)	0.00540 (11)	0.00562 (11)	−0.00008 (8)	0.00033 (8)	0.00085 (8)
W2	0.00472 (11)	0.00554 (11)	0.00480 (11)	0.00064 (8)	−0.00001 (8)	−0.00041 (8)
O1	0.0062 (14)	0.0135 (17)	0.0081 (16)	−0.0004 (12)	−0.0012 (12)	−0.0019 (13)
O2	0.0116 (16)	0.0106 (16)	0.0073 (16)	−0.0022 (13)	0.0000 (13)	−0.0007 (13)
O3	0.0128 (17)	0.0134 (18)	0.0149 (19)	0.0023 (14)	0.0071 (14)	0.0062 (14)
O4	0.0184 (19)	0.0141 (18)	0.0118 (18)	−0.0098 (15)	0.0025 (15)	−0.0006 (15)
O5	0.0117 (17)	0.0112 (17)	0.0098 (17)	0.0032 (13)	0.0018 (13)	0.0006 (13)
O6	0.0097 (16)	0.0092 (16)	0.0098 (16)	0.0027 (12)	−0.0009 (13)	−0.0005 (13)

Geometric parameters (Å, º)

Sr1/La1—O6^{i}	2.333 (4)	Sr3/La3—O1^{xi}	3.220 (4)
Sr1/La1—O2	2.438 (4)	Sr3/La3—W2^{xi}	3.4641 (4)
Sr1/La1—O2^{ii}	2.453 (4)	Sr3/La3—W2^{iii}	3.4641 (4)
Sr1/La1—O4^{iii}	2.458 (4)	Sr4/La4—O1	2.607 (4)
Sr1/La1—O5^{iv}	2.728 (4)	Sr4/La4—O1^{vii}	2.607 (4)
Sr1/La1—O3^{iii}	2.765 (5)	Sr4/La4—O1^{xii}	2.607 (4)
Sr1/La1—O3	2.849 (5)	Sr4/La4—O1^{x}	2.607 (4)
Sr1/La1—O1^{iii}	2.861 (4)	Sr4/La4—O4	2.998 (5)
Sr1/La1—Sr2/La2^{v}	3.4446 (6)	Sr4/La4—O4^{xii}	2.998 (5)
Sr1/La1—Sr2/La2^{v}	3.4446 (6)	Sr4/La4—O4^{x}	2.998 (5)
Sr1/La1—W1^{iii}	3.5630 (4)	Sr4/La4—O4^{vii}	2.998 (5)
Sr1/La1—W1	3.6181 (4)	Sr4/La4—O5^{i}	3.131 (4)
Sr2/La2—O3^{vi}	2.470 (4)	Sr4/La4—O5^{xiii}	3.131 (4)
Sr2/La2—O1^{vii}	2.548 (4)	Sr4/La4—O5^{vi}	3.131 (4)
Sr2/La2—O6	2.599 (4)	Sr4/La4—O5^{ix}	3.131 (4)
Sr2/La2—O2^{viii}	2.603 (4)	W1—O3	1.901 (4)
Sr2/La2—O1	2.642 (4)	W1—O3^{xiv}	1.901 (4)
Sr2/La2—O5	2.652 (4)	W1—O6^{ix}	1.930 (4)
Sr2/La2—O5^{vi}	2.704 (4)	W1—O6^{v}	1.930 (4)
Sr2/La2—O4	2.777 (4)	W1—O2	1.934 (4)
Sr2/La2—O4^{vi}	2.877 (5)	W1—O2^{xiv}	1.934 (4)
Sr2/La2—W2^{iii}	3.2790 (4)	W1—Sr1/La1^{xv}	3.5629 (4)
Sr2/La2—W2	3.3549 (4)	W1—Sr1/La1^{vi}	3.5629 (4)
Sr2/La2—Sr1^{viii}	3.4446 (6)	W1—Sr2/La2^{ix}	3.6177 (4)
Sr3/La3—O6^{i}	2.557 (4)	W1—Sr2/La2^{v}	3.6177 (4)
Sr3/La3—O6^{ix}	2.557 (4)	W2—O4^{xii}	1.891 (4)
Sr3/La3—O5^{ix}	2.596 (4)	W2—O4^{vi}	1.891 (4)
Sr3/La3—O5^{i}	2.596 (4)	W2—O1^{xvi}	1.917 (4)
Sr3/La3—O3	2.660 (4)	W2—O1	1.917 (4)
Sr3/La3—O3^{x}	2.660 (4)	W2—O5^{xii}	1.967 (4)
Sr3/La3—O4^{x}	2.773 (4)	W2—O5^{vi}	1.967 (4)
Sr3/La3—O4	2.773 (4)	W2—Sr2/La2^{xii}	3.2790 (4)
Sr3/La3—O1^{iii}	3.220 (4)	W2—Sr2/La2^{vi}	3.2790 (4)
O6^{i}—Sr1/La1—O2	108.65 (13)	W2^{xi}—Sr3/La3—W2^{iii}	114.236 (19)
O6^{i}—Sr1/La1—O2^{ii}	83.84 (13)	O1—Sr4/La4—O1^{vii}	90.189 (10)
O2—Sr1/La1—O2^{ii}	86.10 (14)	O1—Sr4/La4—O1^{xii}	90.189 (10)
O6^{i}—Sr1/La1—O4^{iii}	139.77 (14)	O1^{vii}—Sr4/La4—O1^{xii}	173.41 (17)
O2—Sr1/La1—O4^{iii}	101.40 (14)	O1—Sr4/La4—O1^{x}	173.41 (17)
O2^{ii}—Sr1/La1—O4^{iii}	125.03 (13)	O1^{vii}—Sr4/La4—O1^{x}	90.189 (10)
O6^{i}—Sr1/La1—O5^{iv}	83.02 (13)	O1^{xii}—Sr4/La4—O1^{x}	90.189 (10)
O2—Sr1/La1—O5^{iv}	163.00 (12)	O1—Sr4/La4—O4	63.92 (11)
O2^{ii}—Sr1/La1—O5^{iv}	82.86 (13)	O1^{vii}—Sr4/La4—O4	56.25 (11)
O4^{iii}—Sr1/La1—O5^{iv}	74.87 (14)	O1^{xii}—Sr4/La4—O4	118.30 (11)
O6^{i}—Sr1/La1—O3^{iii}	146.51 (13)	O1^{x}—Sr4/La4—O4	121.40 (11)
O2—Sr1/La1—O3^{iii}	74.94 (12)	O1—Sr4/La4—O4^{xii}	56.25 (11)

O2^{ii}—Sr1/La1—O3^{iii}	62.93 (12)	O1^{vii}—Sr4/La4—O4^{xii}	121.40 (11)
O4^{iii}—Sr1/La1—O3^{iii}	66.83 (13)	O1^{xii}—Sr4/La4—O4^{xii}	63.92 (11)
O5^{iv}—Sr1/La1—O3^{iii}	88.51 (12)	O1^{x}—Sr4/La4—O4^{xii}	118.30 (11)
O6^{i}—Sr1/La1—O3	89.34 (13)	O4—Sr4/La4—O4^{xii}	120.17 (10)
O2—Sr1/La1—O3	60.49 (12)	O1—Sr4/La4—O4^{x}	121.40 (11)
O2^{ii}—Sr1/La1—O3	141.63 (12)	O1^{vii}—Sr4/La4—O4^{x}	118.30 (11)
O4^{iii}—Sr1/La1—O3	82.66 (13)	O1^{xii}—Sr4/La4—O4^{x}	56.25 (11)
O5^{iv}—Sr1/La1—O3	133.77 (12)	O1^{x}—Sr4/La4—O4^{x}	63.92 (11)
O3^{iii}—Sr1/La1—O3	118.90 (13)	O4—Sr4/La4—O4^{x}	89.71 (17)
O6^{i}—Sr1/La1—O1^{iii}	73.37 (12)	O4^{xii}—Sr4/La4—O4^{x}	120.17 (10)
O2—Sr1/La1—O1^{iii}	123.73 (12)	O1—Sr4/La4—O4^{vii}	118.30 (11)
O2^{ii}—Sr1/La1—O1^{iii}	146.75 (12)	O1^{vii}—Sr4/La4—O4^{vii}	63.92 (11)
O4^{iii}—Sr1/La1—O1^{iii}	67.80 (12)	O1^{xii}—Sr4/La4—O4^{vii}	121.40 (11)
O5^{iv}—Sr1/La1—O1^{iii}	70.80 (11)	O1^{x}—Sr4/La4—O4^{vii}	56.25 (11)
O3^{iii}—Sr1/La1—O1^{iii}	133.60 (11)	O4—Sr4/La4—O4^{vii}	120.17 (10)
O3—Sr1/La1—O1^{iii}	63.35 (11)	O4^{xii}—Sr4/La4—O4^{vii}	89.71 (17)
Sr2/La2^{v}—Sr1/La1—W1	61.565 (10)	O4^{x}—Sr4/La4—O4^{vii}	120.17 (10)
W1^{iii}—Sr1/La1—W1	107.502 (10)	O1—Sr4/La4—O5^{i}	117.41 (11)
O3^{vi}—Sr2/La2—O1^{vii}	143.76 (14)	O1^{vii}—Sr4/La4—O5^{i}	56.35 (11)
O3^{vi}—Sr2/La2—O6	137.69 (13)	O1^{xii}—Sr4/La4—O5^{i}	117.90 (11)
O1^{vii}—Sr2/La2—O6	74.95 (12)	O1^{x}—Sr4/La4—O5^{i}	68.03 (11)
O3^{vi}—Sr2/La2—O2^{viii}	77.47 (13)	O4—Sr4/La4—O5^{i}	53.49 (10)
O1^{vii}—Sr2/La2—O2^{viii}	127.58 (12)	O4^{xii}—Sr4/La4—O5^{i}	173.65 (10)
O6—Sr2/La2—O2^{viii}	60.75 (12)	O4^{x}—Sr4/La4—O5^{i}	62.02 (10)
O3^{vi}—Sr2/La2—O1	71.74 (13)	O4^{vii}—Sr4/La4—O5^{i}	94.03 (11)
O1^{vii}—Sr2/La2—O1	90.70 (17)	O1—Sr4/La4—O5^{xiii}	117.90 (11)
O6—Sr2/La2—O1	140.44 (12)	O1^{vii}—Sr4/La4—O5^{xiii}	117.41 (11)
O2^{viii}—Sr2/La2—O1	141.44 (12)	O1^{xii}—Sr4/La4—O5^{xiii}	68.03 (11)
O3^{vi}—Sr2/La2—O5	101.06 (13)	O1^{x}—Sr4/La4—O5^{xiii}	56.35 (11)
O1^{vii}—Sr2/La2—O5	63.69 (12)	O4—Sr4/La4—O5^{xiii}	173.65 (10)
O6—Sr2/La2—O5	80.29 (12)	O4^{xii}—Sr4/La4—O5^{xiii}	62.02 (10)
O2^{viii}—Sr2/La2—O5	81.63 (12)	O4^{x}—Sr4/La4—O5^{xiii}	94.03 (11)
O1—Sr2/La2—O5	126.30 (12)	O4^{vii}—Sr4/La4—O5^{xiii}	53.49 (10)
O3^{vi}—Sr2/La2—O5^{vi}	118.64 (12)	O5^{i}—Sr4/La4—O5^{xiii}	124.29 (9)
O1^{vii}—Sr2/La2—O5^{vi}	76.11 (12)	O1—Sr4/La4—O5^{vi}	56.35 (11)
O6—Sr2/La2—O5^{vi}	78.82 (12)	O1^{vii}—Sr4/La4—O5^{vi}	68.03 (11)
O2^{viii}—Sr2/La2—O5^{vi}	117.51 (12)	O1^{xii}—Sr4/La4—O5^{vi}	117.41 (11)
O1—Sr2/La2—O5^{vi}	61.87 (12)	O1^{x}—Sr4/La4—O5^{vi}	117.90 (11)
O5—Sr2/La2—O5^{vi}	138.23 (9)	O4—Sr4/La4—O5^{vi}	94.03 (11)
O3^{vi}—Sr2/La2—O4	83.96 (13)	O4^{xii}—Sr4/La4—O5^{vi}	53.49 (10)
O1^{vii}—Sr2/La2—O4	59.86 (12)	O4^{x}—Sr4/La4—O5^{vi}	173.65 (10)
O6—Sr2/La2—O4	128.74 (12)	O4^{vii}—Sr4/La4—O5^{vi}	62.02 (10)
O2^{viii}—Sr2/La2—O4	132.50 (13)	O5^{i}—Sr4/La4—O5^{vi}	124.29 (9)
O1—Sr2/La2—O4	66.80 (12)	O5^{xiii}—Sr4/La4—O5^{vi}	82.71 (14)
O5—Sr2/La2—O4	59.51 (12)	O1—Sr4/La4—O5^{ix}	68.03 (11)
O5^{vi}—Sr2/La2—O4	109.81 (13)	O1^{vii}—Sr4/La4—O5^{ix}	117.90 (11)
O3^{vi}—Sr2/La2—O4^{vi}	64.87 (13)	O1^{xii}—Sr4/La4—O5^{ix}	56.35 (11)
O1^{vii}—Sr2/La2—O4^{vi}	132.31 (11)	O1^{x}—Sr4/La4—O5^{ix}	117.41 (11)

O6—Sr2/La2—O4^{vi}	104.51 (12)	O4—Sr4/La4—O5^{ix}	62.02 (10)
O2^{viii}—Sr2/La2—O4^{vi}	87.33 (12)	O4^{xii}—Sr4/La4—O5^{ix}	94.03 (11)
O1—Sr2/La2—O4^{vi}	58.90 (11)	O4^{x}—Sr4/La4—O5^{ix}	53.49 (10)
O5—Sr2/La2—O4^{vi}	163.87 (12)	O4^{vii}—Sr4/La4—O5^{ix}	173.65 (10)
O5^{vi}—Sr2/La2—O4^{vi}	57.69 (11)	O5^{i}—Sr4/La4—O5^{ix}	82.71 (14)
O4—Sr2/La2—O4^{vi}	123.12 (9)	O5^{xiii}—Sr4/La4—O5^{ix}	124.29 (9)
W2^{iii}—Sr2/La2—W2	121.613 (13)	O5^{vi}—Sr4/La4—O5^{ix}	124.29 (9)
W2^{iii}—Sr2/La2—Sr1/La1^{viii}	155.754 (16)	O3—W1—O3^{xiv}	180.0
W2—Sr2/La2—Sr1/La1^{viii}	78.905 (11)	O3—W1—O6^{ix}	86.73 (17)
O6^{i}—Sr3/La3—O6^{ix}	90.91 (18)	O3^{xiv}—W1—O6^{ix}	93.27 (17)
O6^{i}—Sr3/La3—O5^{ix}	169.96 (12)	O3—W1—O6^{v}	93.27 (17)
O6^{ix}—Sr3/La3—O5^{ix}	82.12 (12)	O3^{xiv}—W1—O6^{v}	86.73 (17)
O6^{i}—Sr3/La3—O5^{i}	82.12 (12)	O6^{ix}—W1—O6^{v}	180.0 (2)
O6^{ix}—Sr3/La3—O5^{i}	169.96 (12)	O3—W1—O2	88.94 (18)
O5^{ix}—Sr3/La3—O5^{i}	105.66 (18)	O3^{xiv}—W1—O2	91.06 (18)
O6^{i}—Sr3/La3—O3	89.14 (13)	O6^{ix}—W1—O2	94.18 (16)
O6^{ix}—Sr3/La3—O3	60.52 (12)	O6^{v}—W1—O2	85.82 (16)
O5^{ix}—Sr3/La3—O3	93.66 (13)	O3—W1—O2^{xiv}	91.07 (18)
O5^{i}—Sr3/La3—O3	111.89 (12)	O3^{xiv}—W1—O2^{xiv}	88.93 (18)
O6^{i}—Sr3/La3—O3^{x}	60.52 (12)	O6^{ix}—W1—O2^{xiv}	85.82 (16)
O6^{ix}—Sr3/La3—O3^{x}	89.14 (13)	O6^{v}—W1—O2^{xiv}	94.18 (16)
O5^{ix}—Sr3/La3—O3^{x}	111.89 (12)	O2—W1—O2^{xiv}	180.0
O5^{i}—Sr3/La3—O3^{x}	93.66 (13)	Sr1/La1^{xv}—W1—Sr1/La1^{vi}	180.0
O3—Sr3/La3—O3^{x}	137.62 (19)	Sr1/La1^{vi}—W1—Sr1/La1^{vi}	0.0
O6^{i}—Sr3/La3—O4^{x}	116.21 (12)	Sr1/La1^{xv}—W1—Sr1/La1^{xv}	0.0
O6^{ix}—Sr3/La3—O4^{x}	117.76 (12)	Sr1/La1^{vi}—W1—Sr1/La1^{xv}	180.0
O5^{ix}—Sr3/La3—O4^{x}	61.78 (12)	Sr1/La1^{xv}—W1—Sr2/La2^{ix}	114.745 (9)
O5^{i}—Sr3/La3—O4^{x}	72.02 (12)	Sr1/La1^{vi}—W1—Sr2/La2^{ix}	65.255 (9)
O3—Sr3/La3—O4^{x}	154.56 (13)	Sr1/La1^{xv}—W1—Sr2/La2^{ix}	114.745 (9)
O3^{x}—Sr3/La3—O4^{x}	64.19 (13)	Sr1/La1^{xv}—W1—Sr2/La2^{v}	65.255 (9)
O6^{i}—Sr3/La3—O4	117.76 (12)	Sr1/La1^{vi}—W1—Sr2/La2^{v}	114.745 (9)
O6^{ix}—Sr3/La3—O4	116.21 (12)	Sr2/La2^{ix}—W1—Sr2/La2^{v}	180.000 (12)
O5^{ix}—Sr3/La3—O4	72.02 (12)	O4^{xii}—W2—O4^{vi}	180.0 (3)
O5^{i}—Sr3/La3—O4	61.78 (12)	O4^{xii}—W2—O1^{xvi}	91.21 (17)
O3—Sr3/La3—O4	64.19 (13)	O4^{vi}—W2—O1^{xvi}	88.79 (17)
O3^{x}—Sr3/La3—O4	154.56 (13)	O4^{xii}—W2—O1	88.80 (17)
O4^{x}—Sr3/La3—O4	99.40 (19)	O4^{vi}—W2—O1	91.20 (17)
O6^{i}—Sr3/La3—O1^{iii}	64.45 (11)	O1^{xvi}—W2—O1	180.0
O6^{ix}—Sr3/La3—O1^{iii}	115.34 (11)	O4^{xii}—W2—O5^{xii}	88.65 (18)
O5^{ix}—Sr3/La3—O1^{iii}	125.14 (11)	O4^{vi}—W2—O5^{xii}	91.35 (18)
O5^{i}—Sr3/La3—O1^{iii}	55.05 (11)	O1^{xvi}—W2—O5^{xii}	90.08 (16)
O3—Sr3/La3—O1^{iii}	60.43 (11)	O1—W2—O5^{xii}	89.92 (16)
O3^{x}—Sr3/La3—O1^{iii}	119.46 (11)	O4^{xii}—W2—O5^{vi}	91.35 (18)
O4^{x}—Sr3/La3—O1^{iii}	126.84 (11)	O4^{vi}—W2—O5^{vi}	88.65 (18)
O4—Sr3/La3—O1^{iii}	53.37 (11)	O1^{xvi}—W2—O5^{vi}	89.92 (16)
O6^{i}—Sr3/La3—O1^{xi}	115.34 (11)	O1—W2—O5^{vi}	90.08 (16)
O6^{ix}—Sr3/La3—O1^{xi}	64.45 (11)	O5^{xii}—W2—O5^{vi}	180.0 (3)
O5^{ix}—Sr3/La3—O1^{xi}	55.05 (11)	Sr2/La2^{xii}—W2—Sr2/La2^{vi}	180.0

O5^{i}—Sr3/La3—O1^{xi}	125.14 (11)	Sr2/La2^{xii}—W2—Sr2/La2^{xii}	0.0
O3—Sr3/La3—O1^{xi}	119.46 (11)	Sr2/La2^{vi}—W2—Sr2/La2^{xii}	180.00 (2)
O3^{x}—Sr3/La3—O1^{xi}	60.43 (11)	Sr2/La2^{vi}—W2—Sr2/La2^{vi}	0.000 (11)
O4^{x}—Sr3/La3—O1^{xi}	53.37 (11)	Sr2/La2^{xii}—W2—Sr2/La2	102.7
O4—Sr3/La3—O1^{xi}	126.84 (11)	Sr2/La2^{vi}—W2—Sr2/La2	77.309 (8)
O1^{iii}—Sr3/La3—O1^{xi}	179.73 (14)	Sr2/La2^{xii}—W2—Sr2/La2	102.691 (8)

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, −*z*+1/2; (ii) −*y*+1/4, *x*+1/4, −*z*+5/4; (iii) *y*+1/4, −*x*+1/4, *z*+1/4; (iv) *y*+1/4, −*x*+3/4, −*z*+3/4; (v) −*x*+1/2, −*y*, *z*+1/2; (vi) −*y*+1/4, *x*−1/4, *z*−1/4; (vii) −*y*+1/4, *x*+1/4, −*z*+1/4; (viii) −*x*+1/2, −*y*, *z*−1/2; (ix) *x*−1/2, *y*, −*z*+1/2; (x) −*x*, −*y*+1/2, *z*; (xi) −*y*−1/4, *x*+1/4, *z*+1/4; (xii) *y*−1/4, −*x*+1/4, −*z*+1/4; (xiii) *y*−1/4, −*x*+3/4, *z*−1/4; (xiv) −*x*, −*y*, −*z*+1; (xv) *y*−1/4, −*x*+1/4, −*z*+5/4; (xvi) −*x*, −*y*, −*z*.