Sr$_9$La$_2$(WO$_6$)$_4$ containing [WO$_6$] octahedra

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A polycrystalline sample of Sr$_9$La$_2$(WO$_6$)$_4$, nonastrontium dilanthanum tetras[orthotungstate(VI)], was prepared by heating a compacted powder mixture of SrCO$_3$, WO$_3$, and La$_2$O$_3$ with an Sr:La:W molar ratio of 9:2:4 at 1473 K. X-ray crystal structure analysis was performed for a Sr$_9$La$_2$(WO$_6$)$_4$ single-crystal grain grown by reheating the sample at 1673 K. Sr$_9$La$_2$(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 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$_9$La$_2$(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 ($\square$).

1. Chemical context

The alkaline-earth (A) rare-earth (Ln) tungstates A$_9$Ln$_2$(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$_9$Gd$_1$Eu$_{0.5}$(WO$_6$)$_4$ (Blaase & Kemmler-Sack, 1983), Ca$_9$Gd$_2$Eu$_2$(WO$_6$)$_4$ (Zeng et al., 2013), Ca$_9$Eu$_2$(WO$_6$)$_4$ (Qin et al., 2012; Zeng et al., 2010), Sr$_9$Eu$_2$(WO$_6$)$_4$ (Qin et al., 2012; Blase & Kemmler-Sack, 1983; Zeng et al., 2010), and Ca$_9$Sr$_2$Eu$_2$(WO$_6$)$_4$ (Zeng et al., 2009). Mn$^{4+}$-doped Sr$_9$Y$_2$(WO$_6$)$_4$ (Shi et al., 2019) and Mn$^{4+}$/Mg$^{2+}$-doped Sr$_9$Y$_2$(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$_9$La$_2$(WO$_6$)$_4$. However, details of the crystal structure, including atom positions, have not been clarified up to now. Sr$_9$La$_2$(WO$_6$)$_4$ compounds prepared by substituting Ln (a rare-earth element) for La in Sr$_9$La$_2$(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$_9$La$_2$(WO$_6$)$_4$ can also be replaced with Ca or Ba. For Ca$_9$Ln$_2$(WO$_6$)$_4$ (Ln = Nd, Sm, Eu, Gd, Tb, Dy), lattice parameters of a tetragonal unit-cell with $11.05 \leq a \leq 11.13$ Å and $16.37 \leq c \leq 16.42$ Å and space group...
I$_4$/a have been reported (Smirnov et al., 1987). Ba$_9$Ln$_2$(WO$_6$)$_4$ compounds (Ln = La, Nd, Sm, Eu) are cubic (8.50 ≤ a ≤ 8.56 Å; Betz et al., 1982). The crystal structures of Sr$_9$La$_2$(WO$_6$)$_4$ [Fm$ar{3}$, a = 16.47013 (6) Å] and Ba$_9$La$_2$(WO$_6$)$_4$ [Fm$ar{3}$, a = 17.12339 (15) Å] have been fully analyzed (Ijdo et al., 2016). However, atomic positions for the tetragonal structures of Ca$_9$Ln$_3$(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$_9$La$_2$(WO$_6$)$_4$.

2. Structural commentary

The unit-cell parameters of Sr$_9$La$_2$(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$_9$La$_2$(WO$_6$)$_4$. W1 (multiplicity and Wyckoff letter 8d with site symmetry T) and W2 (8c, T) 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: 1.955 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, 4...) are 0.6384/0.3616 (19), 0.8913/0.1087 (18), 0.9480/0.052 (4), and 0.985/0.015 (7), respectively. The interatomic distances between (Sr/La) and O and the coordination numbers of the cations are

### Table 1

| Symmetry code | Selected bond lengths (Å) |
|---------------|---------------------------|
| i) x-y-z | Sr1/La1—O6$^*$ 2.333 (4) |
| ii) y+z+x | Sr3/La3—O1$^*$ 3.220 (4) |
| iii) x+y+z | Sr1/La1—O2 2.438 (4) |
| i) y+x+z | Sr1/La1—O2 2.438 (4) |
| iv) y+x+z | Sr1/La2—O4 2.453 (4) |
| v) y+x+z | Sr1/La4—O1$^*$ 2.607 (4) |
| vi) z+x+y | Sr1/La1—O4$^*$ 2.458 (4) |
| vii) z+x+y | Sr1/La3—O5$^*$ 2.728 (4) |
| viii) z+y+x | Sr1/La1—O5$^*$ 2.765 (5) |
| (iv) y+x+z | Sr1/La3—O5$^*$ 2.784 (5) |
| (v) y+x+z | Sr1/La4—O4$^*$ 2.861 (4) |
| (vii) z+x+y | Sr1/La2—O6 2.849 (5) |
| (viii) z+y+x | Sr1/La2—O6 2.877 (4) |
| (ix) x+y+z | Sr1/La1—O3 2.652 (4) |
| (x) x+y+z | Sr2/La2—O6 2.603 (4) |
| (xi) x+y+z | Sr2/La2—O6 2.654 (4) |
| (xii) x+y+z | Sr2/La2—O5 2.704 (4) |
| (xiii) x+y+z | Sr2/La2—O5 2.877 (4) |
| (xiv) x+y+z | Sr2/La2—O4$^*$ 2.877 (5) |
| (xv) x+y+z | Sr2/La2—O4$^*$ 2.877 (5) |
| (xvi) x+y+z | Sr2/La2—O4$^*$ 2.677 (4) |
| (xvii) x+y+z | Sr2/La2—O4$^*$ 2.677 (4) |
| (xviii) x+y+z | Sr2/La2—O4$^*$ 2.677 (4) |
| (xix) x+y+z | Sr2/La2—O4$^*$ 2.677 (4) |
| (xx) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxi) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxii) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxiii) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxiv) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxv) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxvi) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxvii) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxviii) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxix) x+y+z | Sr3/La3—O6 2.654 (4) |
| (xxx) x+y+z | Sr3/La3—O6 2.654 (4) |

Symmetry codes: (i) –x+y+z, –y+z, –z+x; (ii) –x+y+z, –y+z, –z+x; (iii) x+y+z, x+y+z, x+y+z; (iv) y+z+x, y+z+x, y+z+x; (v) y+z+x, y+z+x, y+z+x; (vi) y+z+x, y+z+x, y+z+x; (vii) z+x+y, z+x+y, z+x+y; (viii) z+x+y, z+x+y, z+x+y; (ix) –x+y+z, –x+y+z, –x+y+z; (x) –x+y+z, –x+y+z, –x+y+z; (xi) –x+y+z, –x+y+z, –x+y+z; (xii) –x+y+z, –x+y+z, –x+y+z; (xiii) –x+y+z, –x+y+z, –x+y+z; (xiv) –x+y+z, –x+y+z, –x+y+z; (xv) –x+y+z, –x+y+z, –x+y+z; (xvi) –x+y+z, –x+y+z, –x+y+z; (xvii) –x+y+z, –x+y+z, –x+y+z; (xviii) –x+y+z, –x+y+z, –x+y+z; (xix) –x+y+z, –x+y+z, –x+y+z; (xx) –x+y+z, –x+y+z, –x+y+z; (xxi) –x+y+z, –x+y+z, –x+y+z; (xxii) –x+y+z, –x+y+z, –x+y+z; (xxiii) –x+y+z, –x+y+z, –x+y+z; (xxiv) –x+y+z, –x+y+z, –x+y+z; (xxv) –x+y+z, –x+y+z, –x+y+z; (xxvi) –x+y+z, –x+y+z, –x+y+z; (xxvii) –x+y+z, –x+y+z, –x+y+z; (xxviii) –x+y+z, –x+y+z, –x+y+z; (xxix) –x+y+z, –x+y+z, –x+y+z; (xxx) –x+y+z, –x+y+z, –x+y+z;

Figure 1

The principal building units in the crystal structure of Sr$_9$La$_2$(WO$_6$)$_4$, with displacement ellipsoids drawn at the 99% probability level. Symmetry codes refer to Table 1.
3. Synthesis and crystallization

Raw powdered materials of SrCO₃ (Hakushin Chemical Laboratory, 98%), WO₃ (Furuuchi Chemical, 99.99%), and La₂O₃ (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-crystal line 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 Sr₉La₂(WO₆)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 9.1 (1): 1.9 (1): 4.0 (1): 24.0 (2) calculated from the composition is consistent with the chemical formula Sr₉La₂(WO₆)₄.

Table 2
Experimental details.

| Crystal data | Sr₉La₂(WO₆)₄ |
|--------------|--------------|
| Chemical formula | Sr₉La₂(WO₆)₄ |
| M_r | 2185.80 |
| Crystal system, space group | Tetragonal, I₄₁/a |
| Temperature (K) | 300 |
| a, c (Å) | 11.6365 (3), 16.3040 (4) |
| V (Å³) | 2207.69 (13) |
| Z | 4 |
| Radiation type | Mo Kα |
| µ (mm⁻¹) | 46.16 |
| Crystal size (mm) | 0.05 x 0.04 x 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 > 2σ(I)] reflections | 62981, 2106, 1972 |
| R(int) | 0.048 |
| (sinθ/λ)max (Å⁻¹) | 0.770 |

Refinement

| R[F² > 2σ(F²)], wR(F²), S | 0.025, 0.046, 1.37 |
| No. of reflections | 2106 |
| No. of parameters | 97 |
| No. of restraints | 1 |
| Δρmax, Δρmin (e Å⁻³) | 1.14, −1.50 |

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

Nonastraontium dilanthanum tetrakis[orthotungstate(VI)]

Crystal data
Sr$_9$La$_2$(WO$_6$)$_4$  $D_a = 6.576$ Mg m$^{-3}$
$M_r = 2185.80$  Mo Kα radiation, $\lambda = 0.71073$ Å
Tetragonal, $I4_1/a$  Cell parameters from 9792 reflections
$a = 11.6365$ (3) Å  $\theta = 3.5$–$33.2^\circ$
$c = 16.3040$ (4) Å  $\mu = 46.16$ mm$^{-1}$
$V = 2207.69$ (13) Å$^3$  $T = 300$ K
$Z = 4$  Granular, translucent colourless
$F(000) = 3776$  0.05 × 0.04 × 0.03 mm

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

Refinement
Refinement on $F^2$ $w = 1/[\sigma(F_c^2) + 62.4087P]$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$ where $P = (F_c^2 + 2F_s^2)/3$
$wR(F^2) = 0.046$ $\langle\Delta/\sigma\rangle_{\text{max}} = 0.001$
$S = 1.37$ $\Delta \rho_{\text{max}} = 1.14$ e Å$^{-3}$
2106 reflections $\Delta \rho_{\text{min}} = -1.50$ e Å$^{-3}$
97 parameters Extinction correction: SHELXL-2014/7
1 restraint (Sheldrick, 2015b),
$F^2 = kF(0) + [0.001xF(0)^2]/\sin(2\theta)]^{1/4}$
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     | \(U_{	ext{iso}}^{2}\)/\(U_{	ext{eq}}^{2}\) | 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)**

|    | \(U_{11}^{3}\) | \(U_{22}^{3}\) | \(U_{33}^{3}\) | \(U_{12}^{3}\) | \(U_{13}^{3}\) | \(U_{23}^{3}\) |
|----|----------------|----------------|----------------|----------------|----------------|----------------|
| 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) | −0.0010 (12) | −0.00012 (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 | 2.333 (4) | Sr3/La3—O1 | 3.220 (4) |
| Sr1/La1—O2 | 2.438 (4) | Sr3/La3—W2 | 3.4641 (4) |
| Sr1/La1—O2" | 2.453 (4) | Sr3/La3—W11 | 3.4641 (4) |
| Sr1/La1—O4" | 2.458 (4) | Sr4/La4—O1 | 2.607 (4) |
| Sr1/La1—O5" | 2.728 (4) | Sr4/La4—O11vii | 2.607 (4) |
| Sr1/La1—O3" | 2.765 (5) | Sr4/La4—O11vii | 2.607 (4) |
| Sr1/La1—O1"11i | 2.849 (5) | Sr4/La4—O1xv | 2.607 (4) |
| Sr1/La1—O5iv | 2.728 (4) | Sr4/La4—O4 | 2.998 (5) |
| Sr1/La1—Sr2/La2"11vi | 3.4446 (6) | Sr4/La4—O4xiv | 2.998 (5) |
| Sr1/La1—Sr2/La2"11vi | 3.4446 (6) | Sr4/La4—O4xvii | 2.998 (5) |
| Sr1/La1—W1"8i | 3.5630 (4) | Sr4/La4—O5i | 3.131 (4) |
| Sr1/La1—W1 | 3.6181 (4) | Sr4/La4—O5xvii | 3.131 (4) |
| Sr2/La2—O3"vi | 2.470 (4) | Sr4/La4—O5xvi | 3.131 (4) |
| Sr2/La2—O1"12i | 2.548 (4) | Sr4/La4—O5ix | 3.131 (4) |
| Sr2/La2—O6 | 2.599 (4) | Sr4/La4—O5x | 3.131 (4) |
| Sr2/La2—O2"12i | 2.603 (4) | W1—O3 | 1.901 (4) |
| Sr2/La2—O1 | 2.642 (4) | W1—O3xvi | 1.901 (4) |
| Sr2/La2—O5 | 2.652 (4) | W1—O6v | 1.930 (4) |
| Sr2/La2—O5" | 2.704 (4) | W1—O6v | 1.930 (4) |
| Sr2/La2—O4 | 2.777 (4) | W1—O2 | 1.934 (4) |
| Sr2/La2—O4" | 2.877 (5) | W1—O2xvi | 1.934 (4) |
| Sr2/La2—W2 | 3.2790 (4) | W1—Sr1/La1|xvi | 3.5629 (4) |
| Sr2/La2—W2 | 3.3549 (4) | W1—Sr1/La1vi | 3.5629 (4) |
| Sr2/La2—Sr1"12iii | 3.4446 (6) | W1—Sr2/La2xiv | 3.6177 (4) |
| Sr3/La3—O6 | 2.557 (4) | W1—Sr2/La2xvii | 3.6177 (4) |
| Sr3/La3—O6" | 2.557 (4) | W2—O4xivii | 1.891 (4) |
| Sr3/La3—O5" | 2.596 (4) | W2—O4xiv | 1.891 (4) |
| Sr3/La3—O5" | 2.596 (4) | W2—O1xvii | 1.917 (4) |
| Sr3/La3—O3 | 2.660 (4) | W2—O1 | 1.917 (4) |
| Sr3/La3—O3" | 2.660 (4) | W2—O5xvii | 1.967 (4) |
| Sr3/La3—O4" | 2.773 (4) | W2—O5vi | 1.967 (4) |
| Sr3/La3—O4" | 2.773 (4) | W2—Sr2/La2xviiii | 3.2790 (4) |
| Sr3/La3—O1"11i | 3.220 (4) | W2—Sr2/La2xi | 3.2790 (4) |

O6—Sr1/La1—O2 108.65 (13) W2xvi—Sr3/La3—W2xvi 114.236 (19)
O6—Sr1/La1—O2"iv 83.84 (13) O1—Sr4/La4—O1vii 90.189 (10)
O2—Sr1/La1—O2v 86.10 (14) O1—Sr4/La4—O1xvi 90.189 (10)
O6—Sr1/La1—O4"iv 139.77 (14) O1vii—Sr4/La4—O1xvi 173.41 (17)
O2—Sr1/La1—O4"iv 101.40 (14) O1—Sr4/La4—O1xxi 173.41 (17)
O2v—Sr1/La1—O4"iv 125.03 (13) O1vii—Sr4/La4—O1xvi 90.189 (10)
O6—Sr1/La1—O5"v 83.02 (13) O1xvi—Sr4/La4—O1xvi 90.189 (10)
O2—Sr1/La1—O5"v 163.00 (12) O1—Sr4/La4—O4 63.92 (11)
O2v—Sr1/La1—O5"v 82.86 (13) O1vii—Sr4/La4—O4 56.25 (11)
O4iv—Sr1/La1—O5"v 74.87 (14) O1vi—Sr4/La4—O4 118.30 (11)
O6—Sr1/La1—O3"iv 146.51 (13) O1v—Sr4/La4—O4 121.40 (11)
O2—Sr1/La1—O3"iv 74.94 (12) O1—Sr4/La4—O4xvii 56.25 (11)
| Bond                  | Angle (°) (σ) | Bond                  | Angle (°) (σ) |
|----------------------|--------------|----------------------|--------------|
| O2ii—Sr1/La1—O3iii   | 62.93 (12)   | O1—Sr4/La4—O4vi     | 121.40 (11)  |
| O4ii—Sr1/La1—O3iii  | 66.83 (13)   | O1ii—Sr4/La4—O4vi   | 63.92 (11)   |
| O5vi—Sr1/La1—O3iii  | 88.51 (12)   | O1—Sr4/La4—O4vi     | 118.30 (11)  |
| O6—Sr1/La1—O3       | 89.34 (13)   | O4—Sr4/La4—O4vi     | 120.17 (10)  |
| O2—Sr1/La1—O3—O3    | 60.49 (12)   | O1—Sr4/La4—O4vi     | 121.40 (11)  |
| O2ii—Sr1/La1—O3—O3  | 141.63 (12)  | O1ii—Sr4/La4—O4vi   | 63.92 (11)   |
| O4ii—Sr1/La1—O3—O3  | 82.66 (13)   | O4vi—Sr4/La4—O4vi   | 118.30 (11)  |
| O5vi—Sr1/La1—O3—O3  | 133.77 (12)  | O1—Sr4/La4—O4vi     | 120.17 (10)  |
| O3iii—Sr1/La1—O3—O3 | 118.90 (13)  | O4—Sr4/La4—O4vi     | 63.92 (11)   |
| O6—Sr1/La1—O1—O1    | 73.37 (12)   | O1vi—Sr4/La4—O4vi   | 63.92 (11)   |
| O2—Sr1/La1—O1—O1    | 123.73 (12)  | O4vi—Sr4/La4—O4vi   | 120.17 (10)  |
| O2—Sr1/La1—O1—O1    | 146.75 (12)  | O1—Sr4/La4—O4vi     | 120.17 (10)  |
| O4vi—Sr1/La1—O1—O1  | 67.80 (12)   | O4—Sr4/La4—O4vi     | 120.17 (10)  |
| O5vi—Sr1/La1—O1—O1  | 70.80 (11)   | O1—Sr4/La4—O4vi     | 53.49 (10)   |
| O3iii—Sr1/La1—O1—O1 | 133.60 (11)  | O4vi—Sr4/La4—O4vi   | 173.65 (10)  |
| O3—Sr1/La1—O1—O1    | 63.35 (11)   | O1—Sr4/La4—O5i      | 117.41 (11)  |
| Sr2/La2—Sr1/La1—W1   | 61.565 (10)  | O1vi—Sr4/La4—O5i    | 56.35 (11)   |
| W1—Sr1/La1—W1        | 107.502 (10) | O1—Sr4/La4—O5i      | 117.41 (11)  |
| O3vi—Sr2/La2—O1vi   | 143.76 (14)  | O1—Sr4/La4—O5i      | 117.90 (11)  |
| O3vi—Sr2/La2—O6vi   | 137.69 (13)  | O1vi—Sr4/La4—O5i    | 117.90 (11)  |
| O1vi—Sr2/La2—O6vi   | 74.95 (12)   | O1—Sr4/La4—O5i      | 117.41 (11)  |
| O3vi—Sr2/La2—O2viii  | 77.47 (13)   | O4vi—Sr4/La4—O5i    | 68.03 (11)   |
| O1vi—Sr2/La2—O2viii  | 127.58 (12)  | O1—Sr4/La4—O5i      | 120.17 (10)  |
| O6—Sr2/La2—O2vi     | 120.17 (10)  | O4vi—Sr4/La4—O5i    | 53.49 (10)   |
| O3vi—Sr2/La2—O1     | 63.96 (12)   | O1—Sr4/La4—O5i      | 173.65 (10)  |
| O6—Sr2/La2—O2—O5    | 80.29 (12)   | O4vi—Sr4/La4—O5i    | 94.03 (11)   |
| O2—Sr2/La2—O1—O1    | 140.44 (12)  | O5—Sr4/La4—O5i      | 124.29 (9)   |
| O1vi—Sr2/La2—O5     | 101.06 (13)  | O1—Sr4/La4—O5i      | 53.49 (10)   |
| O6—Sr2/La2—O5—O5    | 63.69 (12)   | O4vi—Sr4/La4—O5i    | 124.29 (9)   |
| O2—Sr2/La2—O5—O5    | 81.63 (12)   | O1—Sr4/La4—O5i      | 63.92 (11)   |
| O1—Sr2/La2—O5—O5    | 126.30 (12)  | O5vi—Sr4/La4—O5i    | 124.29 (9)   |
| O3vi—Sr2/La2—O5vi   | 118.64 (12)  | O5—Sr4/La4—O5i      | 63.92 (11)   |
| O1vi—Sr2/La2—O5vi   | 76.11 (12)   | O1—Sr4/La4—O5i      | 117.90 (11)  |
| O6—Sr2/La2—O5vi     | 78.82 (12)   | O1—Sr4/La4—O5i      | 63.92 (11)   |
| O2—Sr2/La2—O5vi     | 117.51 (12)  | O1—Sr4/La4—O5i      | 117.90 (11)  |
| O1—Sr2/La2—O5vi     | 61.87 (12)   | O4—Sr4/La4—O5i      | 94.03 (11)   |
| O5—Sr2/La2—O5vi     | 138.23 (9)   | O4—Sr4/La4—O5i      | 124.29 (9)   |
| O3vi—Sr2/La2—O4vii  | 83.96 (13)   | O5—Sr4/La4—O5i      | 63.92 (11)   |
| O1vi—Sr2/La2—O4vii  | 59.86 (12)   | O5—Sr4/La4—O5i      | 124.29 (9)   |
| O6—Sr2/La2—O4vii    | 128.74 (12)  | O5—Sr4/La4—O5i      | 62.02 (10)   |
| O2—Sr2/La2—O4vii    | 132.50 (13)  | O5—Sr4/La4—O5i      | 94.03 (11)   |
| O1—Sr2/La2—O4vii    | 66.80 (12)   | O5—Sr4/La4—O5i      | 124.29 (9)   |
| O5—Sr2/La2—O4vii    | 59.51 (12)   | O5—Sr4/La4—O5i      | 82.71 (14)   |
| O5vi—Sr2/La2—O4vii  | 109.81 (13)  | O5—Sr4/La4—O5i      | 68.03 (11)   |
| O3vi—Sr2/La2—O4vii  | 64.87 (13)   | O5—Sr4/La4—O5i      | 117.41 (11)  |
| O1vi—Sr2/La2—O4vii  | 132.31 (11)  | O5—Sr4/La4—O5i      | 117.41 (11)  |
O6—Sr2/La2—O4vi 104.51 (12) O4—Sr4/La4—O5ix 62.02 (10)
O2viii—Sr2/La2—O4vi 87.33 (12) O4vi—Sr4/La4—O5ix 94.03 (11)
O1—Sr2/La2—O4vi 58.90 (11) O4v—Sr4/La4—O5ix 53.49 (10)
O5—Sr2/La2—O4vi 163.87 (12) O4vi—Sr4/La4—O5ix 173.65 (10)
O5vi—Sr2/La2—O4vi 57.69 (11) O5—Sr4/La4—O5ix 82.71 (14)
O4—Sr2/La2—O4vi 123.12 (9) O5ii—Sr4/La4—O5ix 124.29 (9)
W2iii—Sr2/La2—W2 121.613 (13) O5vi—Sr4/La4—O5ix 124.29 (9)
W2v—Sr2/La2—Sr1/La1viii 155.754 (16) O3—W1—O3iv 180.0
W2—Sr2/La2—Sr1/La1viii 78.905 (11) O3—W1—O6ix 86.73 (17)
O6vi—Sr3/La3—O6ix 90.91 (18) O3iv—W1—O6ix 93.27 (17)
O6vi—Sr3/La3—O5ix 169.96 (12) O3—W1—O6ix 93.27 (17)
O6vi—Sr3/La3—O5ix 82.12 (12) O3iv—W1—O6ix 86.73 (17)
O6vi—Sr3/La3—O5ix 82.12 (12) O6—W1—O6v 180.0 (2)
O6vi—Sr3/La3—O5i 169.96 (12) O3—W1—O2 86.73 (17)
O5—Sr3/La3—O5i 105.66 (18) O3iv—W1—O2 93.27 (17)
O6vi—Sr3/La3—O3 89.14 (13) O6—W1—O2 94.18 (16)
O6vi—Sr3/La3—O3 60.52 (12) O3—W1—O2 91.07 (18)
O5.,Sr3/La3—O3 93.66 (13) O6—W1—O2 85.82 (15)
O5i—Sr3/La3—O3 111.89 (12) O3iv—W1—O2 88.93 (16)
O6—Sr3/La3—O3 60.52 (12) O6—W1—O2 94.18 (16)
O6i—Sr3/La3—O3x 89.14 (13) O6—W1—O2 180.0
O5vi—Sr3/La3—O3x 82.12 (12) O2—W1—O2 180.0
O5vi—Sr3/La3—O3x 82.12 (12) Sr1/La1vi—W1—Sr1/La1vi 180.0
O5vi—Sr3/La3—O3x 82.12 (12) Sr1/La1vi—W1—Sr2/La2x 114.745 (9)
O5vi—Sr3/La3—O3x 115.34 (11) Sr1/La1vi—W1—Sr2/La2x 65.255 (9)
O5vi—Sr3/La3—O3x 64.45 (11) Sr1/La1vi—W1—Sr2/La2x 114.745 (9)
O5vi—Sr3/La3—O3x 64.45 (11) Sr1/La1vi—W1—Sr2/La2x 65.255 (9)
O5vi—Sr3/La3—O3x 64.45 (11) Sr2/La2v—W1—Sr2/La2x 114.745 (9)
O5vi—Sr3/La3—O3x 115.34 (11) Sr2/La2v—W1—Sr2/La2x 180.0 (12)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O4vi 180.0 (3)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O1xvi 91.21 (17)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O1xvi 88.79 (17)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O1 88.80 (17)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O1 91.20 (17)
O5vi—Sr3/La3—O3x 64.45 (11) O1xvi—W2—O1 180.0
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O5vii 88.65 (18)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O5vii 91.35 (18)
O5vi—Sr3/La3—O3x 64.45 (11) O1xvi—W2—O5vii 90.08 (16)
O5vi—Sr3/La3—O3x 64.45 (11) O1—W2—O5vii 89.92 (16)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O5vii 91.35 (18)
O5vi—Sr3/La3—O3x 64.45 (11) O4vi—W2—O5vii 88.65 (18)
O5vi—Sr3/La3—O3x 64.45 (11) O1xvi—W2—O5vii 89.92 (16)
O5vi—Sr3/La3—O3x 64.45 (11) O1—W2—O5vii 90.08 (16)
O5vi—Sr3/La3—O3x 64.45 (11) O5vi—W2—O5vii 180.0 (3)
O5vi—Sr3/La3—O3x 64.45 (11) Sr2/La2v—W2—Sr2/La2v 180.0

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| Bond                        | Distance (Å)     | Symmetry Code                      |
|-----------------------------|-------------------|-----------------------------------|
| O5i—Sr3/La3—O1xi            | 125.14 (11)       | Sr2/La2xii—W2—Sr2/La2xii         |
| O3—Sr3/La3—O1xi            | 119.46 (11)       | Sr2/La2xiii—W2—Sr2/La2xii        |
| O3x—Sr3/La3—O1xi           | 60.43 (11)        | Sr2/La2xvi—W2—Sr2/La2xii         |
| O4x—Sr3/La3—O1xi           | 53.37 (11)        | Sr2/La2xiii—W2—Sr2/La2xii        |
| O4—Sr3/La3—O1xii           | 126.84 (11)       | Sr2/La2xiii—W2—Sr2/La2xii        |
| O1iii—Sr3/La3—O1xi         | 179.73 (14)       | Sr2/La2xiii—W2—Sr2/La2xii        |

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+1/4, −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.