Crystal structure of the cubic double-perovskite \( \text{Sr}_2\text{Cr}_{0.84}\text{Ni}_{0.09}\text{Os}_{1.07}\text{O}_6 \)

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The crystal structure of the cubic double-perovskite \( \text{Sr}_2\text{Cr}_{0.84}\text{Ni}_{0.09}\text{Os}_{1.07}\text{O}_6 \), grown at high pressure, was solved using intensity data measured at 113 K. The Os site was modelled with a partial Ni occupancy, and the Cr site was modelled with both Os and Ni partial occupancy. The refined structure shows that this cubic form is stable at 113 K.

1. Chemical context

Recently, so called double-perovskites (DP) having \( AB'B''O_6 \) (\( A = \) divalent ions such as alkali earth or Pb, \( B'B'' = 3d/4d/5d \) transition metals) composition have attracted attention in the field of solid-state physics/chemistry due to their potential as materials for applications in, for example, spintronics, multiferroics, and/or magneto-caloric materials. In 1998, \( \text{Sr}_2\text{FeMoO}_6 \), which has the DP structure, was reported as having half-metallic behavior with a high Curie temperature \( (T_C = 420 \text{ K}) \) (Kobayashi et al., 1998). After this discovery, many analogous DP compounds showing half-metallic and ferrimagnetic behavior have been reported (Table 1). The main contributors to the specific physical properties are the electronic states of the \( B' \) and \( B'' \) elements. As an example, \( \text{Sr}_2\text{CrOsO}_6 \), which shows the highest \( T_C \), has its majority-spin orbital empty while the minority-spin orbital is fully occupied. Both \( \text{Cr}^{3+} (3d^3, t_{2g}) \) and \( \text{Os}^{5+} (5d^3, t_{2g}) \) activate primarily for this state (Mandal et al., 2008). To enhance the property, we have introduced other transition metals into the \( B' \) and \( B'' \) sites and examined for the exchange effects of such alternate transition metals at these sites. For this study, the samples were synthesized by high-pressure techniques; this was required to achieve the effective substitution.

2. Structural commentary

The crystal structure of \( \text{Sr}_2\text{Cr}_{0.84}\text{Ni}_{0.09}\text{Os}_{1.07}\text{O}_6 \) has cubic symmetry of space group \( \text{Fm}\overline{3}m \), having one Sr, one Os, one Cr, and one O atom on crystallographically independent sites in the asymmetric unit. It corresponds to the fully Cr-containing end-member \( \text{Sr}_2\text{CrOsO}_6 \) and the low Ni-substituted \( \text{Sr}_2\text{Cr}_{0.75}\text{Ni}_{0.25}\text{OsO}_6 \) (Chen et al., 2020), not the end-member of the Ni side of the composition, \( \text{Sr}_2\text{NiOsO}_6 \), which has tetragonal symmetry \( \text{I}4/\text{m} \) (Macquart et al., 2005), or the high Ni-substituted \( \text{Sr}_2\text{Cr}_{0.50}\text{Ni}_{0.50}\text{OsO}_6 \) (HT: \( \text{I}4/\text{m} \) and LT: \( \text{C}2/m \); Chen et al., 2020).

In the structure (Fig. 1), the transition metals located at both Cr (\( B' \)) and Os (\( B'' \)) sites show elemental disordering...
behavior: 96.1 (13)% Os + 3.8 (13)% Ni at the Os site and 85.5 (3)% Cr + 12.1 (3)% Os + 2.4 (3)% Ni at the Cr site. Both the Cr and Os sites form three-dimensional framework structures connected by corner sharing of the coordination octahedra, having Os—O = 1.926 (4) Å (coordination volume CV = 9.5405 Å³) and Cr—O = 1.987 (4) Å (CV = 10.4516 Å³) (Fig. 1). The Sr atoms, which are twelve coordinate, are located in the voids of the three-dimensional structure, Sr—O = 2.76739 (11) Å (CV: 49.9388 Å³). From this result, the cubic Sr₂Cr₀.₈₄Ni₀.₀₉Os₁.₀₇O₆ structure is shown to be stable down to at least 113K.

3. Synthesis and crystallization

A black-colored single crystal of Sr₂Cr₀.₈₄Ni₀.₀₉Os₁.₀₇O₆ was obtained as a by-product of the synthesis of the polycrystalline Sr₂Cr₁₋ₓNixoO₆ (x = 0.5). The polycrystalline product was synthesized from powders of SrO (99.9%, Strem Chemicals, Inc., USA), CrO₂ (Magtrieve, Sigma-Aldrich Co., USA), NiO (99.97%, High Purity Chemicals Co., Ltd., Japan), OsO₂ [lab-made: Os powder (99.95%, Nanjing Dongrui Platinum Co., Ltd.) was heated at 673 under flowing O₂ gas, the process was repeated three times]. The thoroughly mixed powders (SrO:CrO₂:NiO:OsO₂:KClO₄ = 2:0.5:0.5:1:0.225 mol) were pressed into a pellet and sealed in a Pt capsule. All the processes were carried out in an Ar-filled glove box. A pressure of 6 GPa was continuously applied by a belt-type pressure apparatus (Kobe Steel, Ltd., Japan), the capsule was heated to 1873 K and held at that temperature for 1 h. The temperature was then quenched to room temperature, following which the pressure was gradually released.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. To ensure refinement stability, displacement parameters of disordered atoms on the same sites were constrained and the sums of occupancies were restrained (SHELXL commands EADP and SUMP, respectively.)

Funding information

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Table 1

| Table 1 | Typical half-metallic and ferrimagnetic double perovskites. |
|---------|-------------------------------------------------------------|
| Compound | Sr₂FeMoO₆ | Sr₂CrReO₆ | Sr₂CrMoO₆ | Sr₂FeReO₆ | Sr₂CrWO₆ | Sr₂CrOsO₆ |
| T_c (K)  | Reference                                      |
|---------|-----------------------------------------------|
| 420     | Kobayashi et al. (1998)                        |
| 635     | De Teresa et al. (2005) and Kato et al. (2002) |
| 450     | Morimoto et al. (2000)                         |
| 400     | Kobayashi et al. (1999)                        |
| 390     | Philipp et al. (2003)                          |
|         | Krockenberger et al. (2007) and Morrow (2016)  |

Table 2

| Table 2 | Experimental details. |
|---------|-----------------------|
| Crystal data |                        |
| Chemical formula | Cr₀.₈₄NixoO₆Os₁.₀₇Sr₂ |
| M_r            | 524.37                |
| Crystal system, space group | Cubic, Fm₃m |
| Temperature (K) | 113                  |
| a (Å)          | 7.8269 (3)            |
| V (Å³)         | 479.48 (6)            |
| Z              | 4                     |
| Radiation type | Mo Kα                 |
| µ (mm⁻¹)       | 52.66                 |
| Crystal size (mm) | 0.10 × 0.10 × 0.07 |

| Data collection | Rigaku AFC11 Saturn724+ (4x4 bin mode) |
| Absorption correction | Multi-scan (CrystalClear; Rigaku, 2002) |
| T_min, T_max | 0.056, 0.184 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 3159, 143, 143 |
| R_num | 0.054 |
| (sin θ/λ)_{max} (Å⁻¹) | 1.012 |

| Refinement | |
| R[F² > 2σ(F²)], wR(F²), S | 0.019, 0.047, 1.34 |
| No. of reflections | 143 |
| No. of parameters | 12 |
| No. of restraints | 1 |
| Δρ_{max}, Δρ_{min} (e Å⁻³) | 2.87, -2.25 |

Computer programs: CrystalClear (Rigaku, 2002), SHELXTL2014/5 (Sheldrick, 2015a), SHELXL2018/1 (Sheldrick, 2015b) and VESTA (Momma & Izumi, 2011).
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Computing details

Data collection: CrystalClear (Rigaku, 2002); cell refinement: CrystalClear (Rigaku, 2002); data reduction: CrystalClear (Rigaku, 2002); program(s) used to solve structure: SHELXT2014/5 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/1 (Sheldrick, 2015b); molecular graphics: VESTA (Momma & Izumi, 2011).

(I)

Crystal data

\([	ext{Cr}_{0.84}\text{Ni}_{0.09}\text{Os}_{1.07}\text{Sr}_2}\) \(M_r = 524.37\)

Cubic, \(Fm\bar{3}m\)

\(a = 7.8269(3)\ \text{Å}\)

\(V = 479.48(6)\ \text{Å}^3\)

\(Z = 4\)

\(F(000) = 913\)

\(D_x = 7.264\ \text{Mg}\ \text{m}^{-3}\)

Data collection

Rigaku AFC11 Saturn724+ (4x4 bin mode) diffractometer

Radiation source: Rigaku rotating anode

Confocal monochromator

Detector resolution: 28.5714 pixels mm\(^{-1}\)

dtprofit.ref scans

Absorption correction: multi-scan (CrystalClear; Rigaku, 2002)

\(T_{\text{min}} = 0.056, \ T_{\text{max}} = 0.184\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.019\)

\(wR(F^2) = 0.047\)

\(S = 1.34\)

143 reflections

12 parameters

1 restraint

\(w = 1/[\sigma^2(F_c^2) + (0.0244P)^2 + 3.1506P]\)

where \(P = (F_c^2 + 2F_i^2)/3\)

\((\Delta/\sigma)_{\text{max}} = 0.001\)

\(\Delta\rho_{\text{max}} = 2.87\ \text{e}\ \text{Å}^{-3}\)

\(\Delta\rho_{\text{min}} = -2.25\ \text{e}\ \text{Å}^{-3}\)

Extinction correction: SHELXL-2018/1

(Sheldrick 2015b),

\(F_c^2 = kF_c[1 + 0.001xF_c^2\lambda^2/sin(2\theta)]^{1/4}\)

Extinction coefficient: 0.0047 (6)
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      | \(U_{iso}^{eq}/U_{eq}\) | Occ. (<1) |
|---|--------|--------|--------|--------------------------|-----------|
| Sr| 0.250000 | 0.250000 | 0.250000 | 0.0075 (3)               |           |
| O | 0.500000 | 0.500000 | 0.2461 (5) | 0.0232 (9)              |           |
| Os| 0.500000 | 0.500000 | 0.000000 | 0.00480 (13)           | 0.962 (13)|
| Ni' | 0.500000 | 0.500000 | 0.000000 | 0.00480 (13)           | 0.037 (13)|
| Cr| 0.500000 | 0.500000 | 0.500000 | 0.0065 (3)              | 0.838 (3) |
| Os' | 0.500000 | 0.500000 | 0.500000 | 0.0065 (3)              | 0.112 (3) |
| Ni" | 0.500000 | 0.500000 | 0.500000 | 0.0065 (3)              | 0.050 (3) |

**Atomic displacement parameters (Å²)**

|   | \(U_{11}^{\parallel}\) | \(U_{22}^{\parallel}\) | \(U_{33}^{\parallel}\) | \(U_{12}^{\parallel}\) | \(U_{13}^{\parallel}\) | \(U_{23}^{\parallel}\) |
|---|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Sr| 0.0075 (3)           | 0.0075 (3)           | 0.0075 (3)           | 0.000000             | 0.000000             | 0.000000             |
| O | 0.0309 (14)          | 0.0309 (14)          | 0.0077 (13)          | 0.000000             | 0.000000             | 0.000000             |
| Os| 0.00480 (13)         | 0.00480 (13)         | 0.00480 (13)         | 0.000000             | 0.000000             | 0.000000             |
| Ni' | 0.00480 (13)         | 0.00480 (13)         | 0.00480 (13)         | 0.000000             | 0.000000             | 0.000000             |
| Cr| 0.0065 (3)           | 0.0065 (3)           | 0.0065 (3)           | 0.000000             | 0.000000             | 0.000000             |
| Os' | 0.0065 (3)           | 0.0065 (3)           | 0.0065 (3)           | 0.000000             | 0.000000             | 0.000000             |
| Ni" | 0.0065 (3)           | 0.0065 (3)           | 0.0065 (3)           | 0.000000             | 0.000000             | 0.000000             |

**Geometric parameters (Å, º)**

|   | Sr—Oi | Sr—Oii | Sr—Oiii | Sr—Oiv | O—Ni' | O—Os | O—Ni" | O—Os' | O—Cr |
|---|-------|--------|---------|--------|-------|------|--------|-------|------|
| Sr—Oi | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Ni' | 1.926 (4) |
| Sr—Oii | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Os | 1.926 (4) |
| Sr—Oiii | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Ni" | 1.987 (4) |
| Sr—Oiv | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Os' | 1.987 (4) |
| Sr—O | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Cr | 1.987 (4) |
| Sr—O | 2.7674 (1) | Sr—Oii | 2.7674 (1) | Sr—Oiii | 2.7674 (1) | Sr—Oiv | 2.7674 (1) | O—Cr | 1.987 (4) |

|   | O—Sr—Oii | O—Sr—Oiii | O—Sr—Oiv | O—Sr—O † | O—Sr—O‡ | O—Sr—O † | O—Sr—O‡ | O—Sr—O † | O—Sr—O‡ |
|---|---------|-----------|----------|----------|---------|----------|----------|----------|---------|
| O—Sr—Oii | 58.98 (13) | O—Sr—O † | 119.96 (1) | O—Sr—O † | 178.75 (16) | O—Sr—O † | 58.98 (13) | O—Sr—O † | 119.96 (1) |
| O—Sr—Oiii | 119.96 (1) | O—Sr—O † | 119.96 (1) | O—Sr—O † | 178.75 (16) | O—Sr—O † | 58.98 (13) | O—Sr—O † | 119.96 (1) |
| O—Sr—Oiv | 119.96 (1) | O—Sr—O † | 119.96 (1) | O—Sr—O † | 178.75 (16) | O—Sr—O † | 58.98 (13) | O—Sr—O † | 119.96 (1) |
| O—Sr—O † | 119.96 (1) | O—Sr—O † | 119.96 (1) | O—Sr—O † | 178.75 (16) | O—Sr—O † | 58.98 (13) | O—Sr—O † | 119.96 (1) |
| O—Sr—O‡ | 119.96 (1) | O—Sr—O † | 119.96 (1) | O—Sr—O † | 178.75 (16) | O—Sr—O † | 58.98 (13) | O—Sr—O † | 119.96 (1) |
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 178.75 (16)  | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | Sr—Ni′—Sr            | 70.5         |
| O—Sr—O               | 61.02 (13)   | Sr—Ni′—Sr            | 109.5        |
| O—Sr—O               | 61.02 (13)   | Sr—Ni′—Sr            | 70.5         |
| O—Sr—O               | 90.007 (2)   | Sr—Ni′—Sr            | 109.5        |
| O—Sr—O               | 90.007 (2)   | Sr—Ni′—Sr            | 109.5        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 180.0        |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 90.000 (1)   |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 180.0        |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 178.75 (16)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 90.0         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 180.0        |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 61.02 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 119.996 (1)  | O—Ni′—Sr             | 54.7         |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 90.007 (2)   | O—Ni′—Sr             | 125.3        |
| O—Sr—O               | 58.98 (13)   | O—Ni′—Sr             | 125.3        |

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| Bond                  | Length (Å) | Torsion (°) | Bond                  | Length (Å) | Torsion (°) |
|----------------------|------------|-------------|----------------------|------------|-------------|
| O_{ii}—Sr—O_{xi}     | 119.996 (1)|            | O_{viii}—Cr—Sr_{xx}  | 125.264 (1)|            |
| O_{iii}—Sr—O_{xi}    | 58.98 (13) |            | O_{v}—Cr—Sr_{xx}     | 54.7       |            |
| O_{iv}—Sr—O_{xi}     | 61.02 (13) |            | O_{vi}—Cr—Sr_{xx}    | 54.7       |            |
| O_{v}—Sr—O_{xi}      | 90.007 (2) |            | O_{vii}—Cr—Sr_{xx}   | 54.7       |            |
| O_{vi}—Sr—O_{xi}     | 119.996 (1)|            | O_{viii}—Cr—Sr_{xx}  | 125.3      |            |
| O_{vii}—Sr—O_{xi}    | 61.02 (13) |            | O_{ix}—Cr—Sr_{xx}    | 109.5      |            |
| O_{viii}—Sr—O_{xi}   | 58.98 (13) |            | O_{ix}—Cr—Sr_{xx}    | 109.5      |            |
| O_{ix}—Sr—O_{xi}     | 119.996 (1)|            | O_{x}—Cr—Sr_{xx}     | 54.7       |            |
| O_{i}—Sr—O_{xi}      | 178.75 (16)|           | Ni′—O—Os′            | 180.0      |            |
| Ni′—O—O_{i}          | 0.0        |            | O_{i}—Sr—O_{xi}      | 180.0      |            |
| Os—O—O_{i}           | 180.0      |            | Ni′—O—Cr             | 180.0      |            |
| Ni′—O—Cr             | 0.0        |            | Os—O—Cr             | 180.0      |            |
| Ni′—O—Cr             | 180.0      |            | Ni′—O—S_{xx}         | 180.0      |            |
| O_{i}—Sr—Cr          | 0.0        |            | O_{ii}—O—S_{xx}      | 89.37 (8)  | 90.0        |
| O_{ii}—O—S_{xx}      | 89.37 (8)  |            | O_{iii}—O—S_{xx}     | 89.37 (8)  | 90.0        |
| Ni′—O—Sr             | 90.63 (8)  |            | Cr—O—S_{xx}          | 89.37 (8)  | 90.0        |
| Cr—O—S_{xx}          | 89.37 (8)  |            | O_{i}—O—S_{xx}       | 90.63 (8)  | 90.0        |
| Sr_{xx}—O—Sr_{xx}    | 178.75 (16)|           | Os—O—S_{xx}          | 90.63 (8)  | 90.0        |
| Sr—O—Sr_{xx}         | 89.993 (2) |            | Ni′—O—S_{xx}         | 90.63 (8)  | 90.0        |
| Sr—O—S_{xx}          | 89.993 (2) |            | Ni″—O—S_{xx}         | 90.63 (8)  | 90.0        |
| Ni″—O—S_{xx}         | 90.63 (8)  |            | Ni″—O—Sr_{xx}        | 90.63 (8)  | 90.0        |
| Ni″—O—Sr_{xx}        | 90.63 (8)  |            | Ni″—O—S_{xx}         | 89.37 (8)  | 90.0        |
| Ni′—O—Sr_{xx}        | 89.37 (8)  |            | Ni′—O—S_{xx}         | 89.37 (8)  | 90.0        |
| Ni′—O—S_{xx}         | 89.37 (8)  |            | O_{i}—O—S_{xx}       | 90.63 (8)  | 90.0        |
| O_{i}—O—S_{xx}       | 90.63 (8)  |            | Ni′—O—S_{xx}         | 90.63 (8)  | 90.0        |
| O—O_{iii}            | 90.0       |            | O_{iv}—O—S_{xx}      | 90.37 (8)  | 90.0        |
| O—O_{i}              | 90.0       |            | O_{iv}—O—S_{xx}      | 90.37 (8)  | 90.0        |
| O—O_{xx}             | 90.0       |            | O_{v}—O—S_{xx}       | 90.37 (8)  | 90.0        |
| Bond                  | Angle (°) | Bond                  | Angle (°) |
|-----------------------|-----------|-----------------------|-----------|
| Oviii—Os—Oviii        | 180.0     | O—Os′—Sr             | 54.7      |
| O—Os—Ox              | 90.0      | Oviii—Os′—Srxxii     | 54.7      |
| Ovii—Os—Ox           | 90.0      | O—Os′—Srxxii        | 125.3     |
| Oviii—Os—Ox           | 90.0      | Oviii—Os′—Srxxii    | 54.7      |
| O—Os—Oxiv            | 90.0      | O—Os′—Srxxii       | 125.3     |
| Ovii—Os—Oxiv         | 90.0      | Ovii—Os′—Srxxii   | 54.7      |
| Oxii—Os—Oxiv         | 90.0      | Oxii—Os′—Srxxii  | 125.3     |
| O—Os—Oxv             | 180.0     | O—Os′—Srxxii      | 125.264 (1)|
| Ovii—Os—Oxv          | 90.0      | Ovii—Os′—Srxxii  | 54.7      |
| Oxiii—Os—Oxv         | 90.0      | Oxiii—Os′—Srxxii | 54.7      |
| Oxiv—Os—Oxv          | 90.0      | Oxiv—Os′—Srxxii | 125.3     |
| Oxv—Os—Oxv           | 90.0      | Oxv—Os′—Srxxii | 54.7      |
| Sr—Os—Oxv            | 109.5     | Sr—Os′—Srxxii    | 70.5      |
| Oxvi—Os—Sr           | 70.5      | Oxvi—Os′—Srxxii  | 70.5      |
| Oxv—Os—Sr            | 109.5     | Oxv—Os′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii   | 125.3     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii  | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 109.5     |
| Oxv—Sr               | 70.5      | Oxv—Sr′—Srxxii | 125.3     |
| Sr—Os—Sr             | 70.5      | Sr—Os′—Srxxii | 70.5      |
| Bond | Angle (°) |
|------|----------|
| $\text{O}^{\text{sv}}-\text{Os}-\text{Sr}^{\text{sv}}$ | 54.7 |
| $\text{Sr}^{\text{xi}}-\text{Os}-\text{Sr}^{\text{sv}}$ | 70.5 |
| $\text{Sr}^{\text{sv}}-\text{Os}-\text{Sr}^{\text{sv}}$ | 109.5 |
| $\text{Sr}-\text{Os}-\text{Sr}^{\text{sv}}$ | 180.0 |
| $\text{O}-\text{Os}-\text{Sr}^{\text{xi}}$ | 54.7 |
| $\text{O}^{\text{vii}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 54.7 |
| $\text{O}^{\text{viii}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{ix}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}_{\text{vii}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 54.7 |
| $\text{O}^{\text{xiv}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 180.0 |
| $\text{O}^{\text{xv}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 180.0 |
| $\text{S}^{\text{rxiv}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{Sr}-\text{Os}-\text{Sr}^{\text{xi}}$ | 70.5 |
| $\text{Sr}^{\text{xi}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 109.5 |
| $\text{Sr}^{\text{sv}}-\text{Os}-\text{Sr}^{\text{xi}}$ | 109.5 |
| $\text{O}^{\text{vec}}-\text{Ni}^{\text{iv}}-\text{O}^{\text{vii}}$ | 90.0 |
| $\text{O}^{\text{vec}}-\text{Ni}^{\text{iv}}-\text{O}^{\text{viii}}$ | 90.0 |
| $\text{O}^{\text{vec}}-\text{Ni}^{\text{iv}}-\text{O}^{\text{x}}$ | 90.0 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{O}^{\text{viii}}$ | 90.0 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| $\text{O}^{\text{v}}-\text{Ni}^{\text{iv}}-\text{Sr}^{\text{xi}}$ | 125.3 |
| Bond | Symmetry | Distance |
|------|----------|----------|
| O^{xvi}—Ni′—Sr | 125.3 | O—Ni''—Sr^{xv} | 54.7 |
| O^{xv}—Ni′—Sr | 125.3 | Sr—Ni''—Sr^{xi} | 109.5 |
| Sr^{xvi}—Ni′—Sr | 109.5 | Sr^{xv}—Ni''—Sr^{xv} | 70.5 |
| Sr^{xvi}—Ni′—Sr | 70.5 | Sr^{xv}—Ni''—Sr^{xv} | 70.5 |
| O—Ni′—Sr^{xv} | 54.7 | Sr^{xv}—Ni''—Sr^{xv} | 180.0 |
| O^{xvii}—Ni′—Sr^{xv} | 125.3 | O^{xv}—Ni''—Sr^{xv} | 54.7 |
| O^{xvii}—Ni′—Sr^{xv} | 54.7 | O^{xvii}—Ni''—Sr^{xv} | 54.7 |
| O^{xviii}—Ni′—Sr^{xv} | 125.3 | O^{xvii}—Ni''—Sr^{xv} | 125.3 |
| O^{xviii}—Ni′—Sr^{xv} | 54.7 | O^{xviii}—Ni''—Sr^{xv} | 54.7 |
| Sr—Ni′—Sr^{xv} | 70.5 | O^{xvii}—Ni''—Sr^{xv} | 125.3 |
| Sr^{xvi}—Ni′—Sr^{xv} | 109.5 | O^{xviii}—Ni''—Sr^{xv} | 125.3 |
| Sr—Ni′—Sr^{xv} | 70.5 | Sr^{xv}—Ni''—Sr^{xv} | 70.5 |
| O—Ni′—Sr^{xv} | 125.3 | Sr^{xv}—Ni''—Sr^{xv} | 70.5 |
| O^{xv}—Ni′—Sr^{xv} | 125.3 | Sr^{xv}—Ni''—Sr^{xv} | 70.5 |
| O^{xv}—Ni′—Sr^{xv} | 54.7 | Sr^{xv}—Ni''—Sr^{xv} | 109.5 |

Symmetry codes: (i) x−1/2, y−1/2, z; (ii) y−1/2, z, x−1/2; (iii) y, z, x; (iv) z, x−1/2, y−1/2; (v) z, x, y; (vi) −y+1/2, −z+1/2, −x+1; (vii) −y+1, −z+1/2, −x+1/2; (viii) −z+1/2, −x−1/2, −y+1; (ix) −z+1/2, −x+1, −y+1/2; (x) −z+1/2, −y+1, −x+1/2; (xi) −x+1, −y+1/2, −z+1/2; (xii) x+1/2, y+1/2, z; (xiii) y, z+1/2, x−1/2; (xiv) z+1/2, x, y−1/2; (xv) −x+1, −y+1, −z; (xvi) −x−1/2, −y+1/2, −z; (xvii) −y+1, −z+1, −x+1; (xviii) −z+1, −x+1, −y+1; (xix) −x+1, −y+1, −z+1; (xx) −x+1/2, −y+1/2, −z+1; (xxi) x+1/2, y, z+1/2.