Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of the cubic double-perovskite $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$

Jie Chen,* Yoshihiro Tsujimoto, Alexei A. Belik, Kazunari Yamaura and Yoshitaka Matsushita*

National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan. *Correspondence e-mail: jiechen@gmail.com, Matsushita.Yoshitaka@nims.go.jp

Received 19 July 2022
Accepted 18 October 2022

Edited by S. Parkin, University of Kentucky, USA

Keywords: crystal structure; osmate; oxide; high-pressure synthesis; cubic double perovskite.

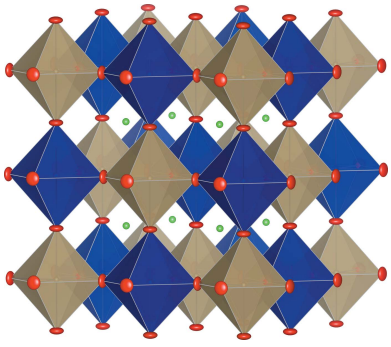
CCDC reference: 2213752

Supporting information: this article has supporting information at journals.iucr.org/e

The crystal structure of the cubic double-perovskite $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$, 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'' = 3*d*/4*d*/5*d* 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, Sr_2FeMoO_6, which has the DP structure, was reported as having half-metallic behavior with a high Curie temperature (T_C = 420 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, Sr_2CrOsO_6, which shows the highest T_C, has its majority-spin orbital empty while the minority-spin orbital is fully occupied. Both Cr^{3+} ($3d^3$, t_{2g^3}) and Os^{5+} ($5d^3$, t_{2g^3}) 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 $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$ has cubic symmetry of space group $Fm\bar{3}m$, 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 Sr_2CrOsO_6 and the low Ni-substituted $Sr_2Cr_{0.75}Ni_{0.25}OsO_6$ (Chen *et al.*, 2020), not the end-member of the Ni side of the composition, Sr_2NiOsO_6, which has tetragonal symmetry $I4/m$ (Macquart *et al.*, 2005), or the high Ni-substituted $Sr_2Cr_{0.50}Ni_{0.50}OsO_6$ (HT: $I4/m$ and LT: $C2/m$; Chen *et al.*, 2020).

In the structure (Fig. 1), the transition metals located at both Cr (B') and Os (B'') sites show elemental disordering

Table 1
Typical half-metallic and ferrimagnetic double perovskites.

Compound	Sr_2FeMoO_6	Sr_2CrReO_6	Sr_2CrMoO_6	Sr_2FeReO_6	Sr_2CrWO_6	Sr_2CrOsO_6
T_C (K)	420	635	450	400	390	725 / 660
Reference	Kobayashi *et al.* (1998)	De Teresa *et al.* (2005) and Kato *et al.* (2002)	Moritomo *et al.* (2000)	Kobayashi *et al.* (1999)	Philipp *et al.* (2003)	Krockenberger *et al.* (2007) and Morrow *et al.* (2016)

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 Å^3) and Cr—O = 1.987 (4) Å (CV = 10.4516 Å^3) (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 Å^3). From this result, the cubic $Sr_2Cr_{0.85}Ni_{0.06}Os_{1.08}O_6$ structure is shown to be stable down to at least 113K.

3. Synthesis and crystallization

A black-colored single crystal of $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$ was obtained as a by-product of the synthesis of the polycrystalline $Sr_2Cr_{1-x}Ni_xOsO_6$ (x = 0.5). The polycrystalline product was synthesized from powders of SrO (99.9%, Strem Chemicals, Inc., USA), CrO_2 (Magtrieve, Sigma-Aldrich Co., USA), NiO (99.97%, High Purity Chemicals Co., Ltd., Japan), OsO_2 [lab-made: Os powder (99.95%, Nanjing Dongrui Platinum Co., Ltd.) was heated at 673 under flowing O_2 gas, the process was repeated three times]. The thoroughly mixed powders (SrO:CrO_2:NiO: OsO_2:$KClO_4$ = 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.

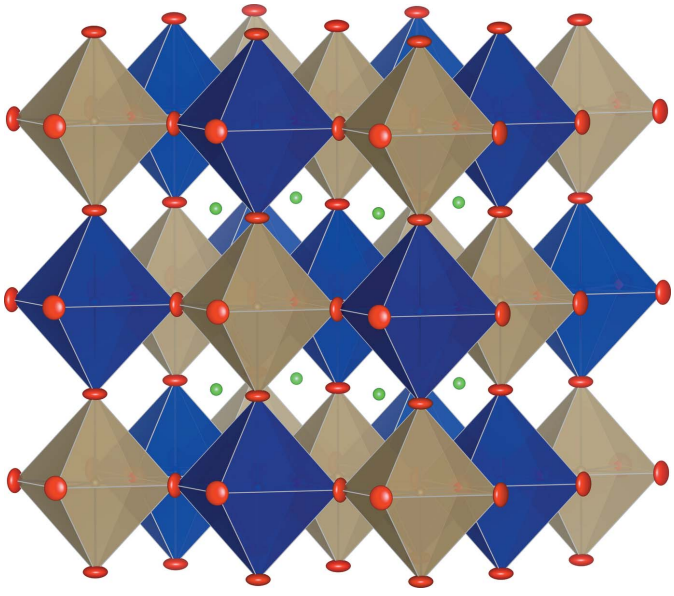


Figure 1
Displacement ellipsoid (probability 50%) and polyhedron view of the cubic double-perovskite $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$. Blue and light-brown polyhedra are CrO_6 and OsO_6, respectively. Red and green ellipsoids are oxygen and Sr, respectively. Figure drawn using *VESTA* (Momma & Izumi, 2011).

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

Funding for this research was provided by: KAKENHI 19H05819 and 22H04601.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Cr_{0.84}Ni_{0.09}O_6Os_{1.07}Sr_2$
M_r	524.37
Crystal system, space group	Cubic, $Fm\bar{3}m$
Temperature (K)	113
a (Å)	7.8269 (3)
V (Å^3)	479.48 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	52.66
Crystal size (mm)	0.10 × 0.10 × 0.07
Data collection	
Diffractometer	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 [$I > 2\sigma(I)$] reflections	3159, 143, 143
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	1.012
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.047, 1.34
No. of reflections	143
No. of parameters	12
No. of restraints	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.87, −2.25

Computer programs: *CrystalClear* (Rigaku, 2002), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*) and *VESTA* (Momma & Izumi, 2011).

References

Chen, J., Wang, X., Hu, Z., Tjeng, L. H., Agrestini, S., Valvidares, M., Chen, K., Nataf, L., Baudelet, F., Nagao, M., Inaguma, Y., Belik, A. A., Tsujimoto, Y., Matsushita, Y., Kolodiazhnyi, T., Sereika, R., Tanaka, M. & Yamaura, K. (2020). *Phys. Rev. B*, **102**, 184418.

De Teresa, J. M., Serrate, D., Ritter, C., Blasco, J., Ibarra, M. R., Morellon, L. & Tokarz, W. (2005). *Phys. Rev. B*, **71**, 092408.

Kato, H., Okuda, T., Okimoto, Y., Tomioka, Y., Takenoya, Y., Ohkubo, A., Kawasaki, M. & Tokura, Y. (2002). *Appl. Phys. Lett.* **81**, 328–330.

Kobayashi, K.-I., Kimura, T., Sawada, H., Terakura, K. & Tokura, Y. (1998). *Nature*, **395**, 677–680.

Kobayashi, K.-I., Kimura, T., Tomioka, Y., Sawada, H., Terakura, K. & Tokura, Y. (1999). *Phys. Rev. B*, **59**, 11159–11162.

Krockenberger, Y., Mogare, K., Reehuis, M., Tovar, M., Jansen, G., Vaitheeswaran, V., Kanchana, F., Bultmark, A., Delin, F., Wilhelm, A., Rogalev, A., Winkler, A. & Alff, L. (2007). *Phys. Rev. B*, **75**, 020404R).

Macquart, R., Kim, S.-J., Gemmill, W. R., Stalick, J. K., Lee, Y. J., Vogt, T. & zur Loye, H. C. (2005). *Inorg. Chem.* **44**, 9676–9683.

Mandal, T. K., Felser, C., Greenblatt, M. & Kübler, J. (2008). *Phys. Rev. B*, **78**, 134431.

Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.

Moritomo, Y., Xu, S., Machida, A., Akimoto, T., Nishibori, E., Takata, M. & Sakata, M. (2000). *Phys. Rev. B*, **61**, R7827–R7830.

Morrow, R., Soliz, J. R., Hauser, A. J., Gallagher, J. C., Susner, M. A., Sumption, M. D., Aczel, A. A., Yan, J., Yang, F. & Woodward, P. M. (2016). *J. Solid State Chem.* **238**, 46–52.

Philipp, J. B., Majewski, P., Alff, L., Erb, A., Gross, R., Graf, T., Brandt, M. S., Simon, J., Walther, T., Mader, W., Topwal, D. & Sarma, D. D. (2003). *Phys. Rev. B*, **68**, 144431.

Rigaku (2002). *CrystalClear* Rigaku/MSC Inc., The Woodlands, Texas, USA.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

supporting information

Acta Cryst. (2022). E**78**, 1135-1137 [https://doi.org/10.1107/S205698902201012X]

Crystal structure of the cubic double-perovskite $Sr_2Cr_{0.84}Ni_{0.09}Os_{1.07}O_6$

Jie Chen, Yoshihiro Tsujimoto, Alexei A. Belik, Kazunari Yamaura and Yoshitaka Matsushita

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

$Cr_{0.84}Ni_{0.09}O_6Os_{1.07}Sr_2$
M_r = 524.37
Cubic, $Fm\bar{3}m$
a = 7.8269 (3) Å
V = 479.48 (6) Å^3
Z = 4
$F(000)$ = 913
D_x = 7.264 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3313 reflections
θ = 4.5–46.0°
μ = 52.66 mm^{-1}
T = 113 K
Chunk, black
0.10 × 0.10 × 0.07 mm

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_{min} = 0.056, T_{max} = 0.184
3159 measured reflections
143 independent reflections
143 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 46.0°, θ_{min} = 4.5°
h = −15→11
k = −15→11
l = −15→15

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
$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2 + 3.1506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.87 e Å^{-3}
$\Delta\rho_{min}$ = −2.25 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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}*/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}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr	0.0075 (3)	0.0075 (3)	0.0075 (3)	0.000	0.000	0.000
O	0.0309 (14)	0.0309 (14)	0.0077 (13)	0.000	0.000	0.000
Os	0.00480 (13)	0.00480 (13)	0.00480 (13)	0.000	0.000	0.000
Ni′	0.00480 (13)	0.00480 (13)	0.00480 (13)	0.000	0.000	0.000
Cr	0.0065 (3)	0.0065 (3)	0.0065 (3)	0.000	0.000	0.000
Os′	0.0065 (3)	0.0065 (3)	0.0065 (3)	0.000	0.000	0.000
Ni"	0.0065 (3)	0.0065 (3)	0.0065 (3)	0.000	0.000	0.000

Geometric parameters (Å, º)

Sr—O^{i}	2.7674 (1)	Sr—O^{ix}	2.7674 (1)
Sr—O^{ii}	2.7674 (1)	Sr—O^{x}	2.7674 (1)
Sr—O^{iii}	2.7674 (1)	Sr—O^{xi}	2.7674 (1)
Sr—O^{iv}	2.7674 (1)	O—Ni′	1.926 (4)
Sr—O^{v}	2.7674 (1)	O—Os	1.926 (4)
Sr—O	2.7674 (1)	O—Ni"	1.987 (4)
Sr—O^{vi}	2.7674 (1)	O—Os′	1.987 (4)
Sr—O^{vii}	2.7674 (1)	O—Cr	1.987 (4)
Sr—O^{viii}	2.7674 (1)		
O^{i}—Sr—O^{ii}	58.98 (13)	O^{ix}—Ni′—Sr^{xv}	125.3
O^{i}—Sr—O^{iii}	119.996 (1)	O^{xiv}—Ni′—Sr^{xv}	54.7
O^{ii}—Sr—O^{iii}	178.75 (16)	O^{xv}—Ni′—Sr^{xv}	54.7
O^{i}—Sr—O^{iv}	58.98 (13)	Sr^{xii}—Ni′—Sr^{xv}	70.5
O^{ii}—Sr—O^{iv}	58.98 (13)	Sr^{xvi}—Ni′—Sr^{xv}	109.5
O^{iii}—Sr—O^{iv}	119.996 (1)	Sr—Ni′—Sr^{xv}	180.0
O^{i}—Sr—O^{v}	119.996 (1)	Sr^{x}—Ni′—Sr^{xv}	109.5
O^{ii}—Sr—O^{v}	119.996 (1)	O—Ni′—Sr^{xi}	54.7

O^{iii}—Sr—O^{v}	61.02 (13)	O^{vii}—Ni′—Sr^{xi}	54.7
O^{iv}—Sr—O^{v}	178.75 (16)	O^{xiii}—Ni′—Sr^{xi}	125.3
O^{i}—Sr—O	178.75 (16)	O^{ix}—Ni′—Sr^{xi}	125.3
O^{ii}—Sr—O	119.996 (1)	O^{xiv}—Ni′—Sr^{xi}	54.7
O^{iii}—Sr—O	61.02 (13)	O^{xv}—Ni′—Sr^{xi}	125.3
O^{iv}—Sr—O	119.996 (1)	Sr^{xii}—Ni′—Sr^{xi}	70.5
O^{v}—Sr—O	61.02 (13)	Sr^{xvi}—Ni′—Sr^{xi}	109.5
O^{i}—Sr—O^{vi}	61.02 (13)	Sr—Ni′—Sr^{xi}	70.5
O^{ii}—Sr—O^{vi}	90.007 (2)	Sr^{x}—Ni′—Sr^{xi}	109.5
O^{iii}—Sr—O^{vi}	90.007 (2)	Sr^{xv}—Ni′—Sr^{xi}	109.5
O^{iv}—Sr—O^{vi}	119.996 (1)	O^{xvii}—Cr—O^{iii}	180.0
O^{v}—Sr—O^{vi}	58.98 (13)	O^{xvii}—Cr—O^{xviii}	90.000 (1)
O—Sr—O^{vi}	119.996 (1)	O^{iii}—Cr—O^{xviii}	90.0
O^{i}—Sr—O^{vii}	119.996 (1)	O^{xvii}—Cr—O^{v}	90.0
O^{ii}—Sr—O^{vii}	90.007 (2)	O^{iii}—Cr—O^{v}	90.000 (1)
O^{iii}—Sr—O^{vii}	90.007 (2)	O^{xviii}—Cr—O^{v}	180.0
O^{iv}—Sr—O^{vii}	61.02 (13)	O^{xvii}—Cr—O^{xix}	90.0
O^{v}—Sr—O^{vii}	119.996 (1)	O^{iii}—Cr—O^{xix}	90.0
O—Sr—O^{vii}	58.98 (13)	O^{xviii}—Cr—O^{xix}	90.0
O^{vi}—Sr—O^{vii}	178.75 (16)	O^{v}—Cr—O^{xix}	90.0
O^{i}—Sr—O^{viii}	61.02 (13)	O^{xvii}—Cr—O	90.0
O^{ii}—Sr—O^{viii}	119.996 (1)	O^{iii}—Cr—O	90.0
O^{iii}—Sr—O^{viii}	58.98 (13)	O^{xviii}—Cr—O	90.0
O^{iv}—Sr—O^{viii}	90.007 (2)	O^{v}—Cr—O	90.0
O^{v}—Sr—O^{viii}	90.007 (2)	O^{xix}—Cr—O	180.0
O—Sr—O^{viii}	119.996 (1)	O^{xvii}—Cr—Sr	125.3
O^{vi}—Sr—O^{viii}	61.02 (13)	O^{iii}—Cr—Sr	54.7
O^{vii}—Sr—O^{viii}	119.996 (1)	O^{xviii}—Cr—Sr	125.3
O^{i}—Sr—O^{ix}	119.996 (1)	O^{v}—Cr—Sr	54.7
O^{ii}—Sr—O^{ix}	61.02 (13)	O^{xix}—Cr—Sr	125.3
O^{iii}—Sr—O^{ix}	119.996 (1)	O—Cr—Sr	54.7
O^{iv}—Sr—O^{ix}	90.007 (2)	O^{xvii}—Cr—Sr^{xix}	54.7
O^{v}—Sr—O^{ix}	90.007 (2)	O^{iii}—Cr—Sr^{xix}	125.3
O—Sr—O^{ix}	58.98 (13)	O^{xviii}—Cr—Sr^{xix}	54.7
O^{vi}—Sr—O^{ix}	119.996 (1)	O^{v}—Cr—Sr^{xix}	125.3
O^{vii}—Sr—O^{ix}	58.98 (13)	O^{xix}—Cr—Sr^{xix}	54.7
O^{viii}—Sr—O^{ix}	178.75 (16)	O—Cr—Sr^{xix}	125.3
O^{i}—Sr—O^{x}	90.007 (2)	Sr—Cr—Sr^{xix}	180.0
O^{ii}—Sr—O^{x}	61.02 (13)	O^{xvii}—Cr—Sr^{xi}	125.3
O^{iii}—Sr—O^{x}	119.996 (1)	O^{iii}—Cr—Sr^{xi}	54.7
O^{iv}—Sr—O^{x}	119.996 (1)	O^{xviii}—Cr—Sr^{xi}	54.7
O^{v}—Sr—O^{x}	58.98 (13)	O^{v}—Cr—Sr^{xi}	125.3
O—Sr—O^{x}	90.007 (2)	O^{xix}—Cr—Sr^{xi}	125.264 (1)
O^{vi}—Sr—O^{x}	58.98 (13)	O—Cr—Sr^{xi}	54.7
O^{vii}—Sr—O^{x}	119.996 (1)	Sr—Cr—Sr^{xi}	70.5
O^{viii}—Sr—O^{x}	119.996 (1)	Sr^{xix}—Cr—Sr^{xi}	109.5
O^{ix}—Sr—O^{x}	61.02 (13)	O^{xvii}—Cr—Sr^{xx}	125.3
O^{i}—Sr—O^{xi}	90.007 (2)	O^{iii}—Cr—Sr^{xx}	54.7

O^{ii}—Sr—O^{xi}	119.996 (1)	O^{xviii}—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^{xix}—Cr—Sr^{xx}	54.7
O^{v}—Sr—O^{xi}	119.996 (1)	O—Cr—Sr^{xx}	125.3
O—Sr—O^{xi}	90.007 (2)	Sr—Cr—Sr^{xx}	70.5
O^{vi}—Sr—O^{xi}	119.996 (1)	Sr^{xix}—Cr—Sr^{xx}	109.5
O^{vii}—Sr—O^{xi}	61.02 (13)	Sr^{xi}—Cr—Sr^{xx}	109.5
O^{viii}—Sr—O^{xi}	58.98 (13)	O^{xvii}—Cr—Sr^{xii}	54.7
O^{ix}—Sr—O^{xi}	119.996 (1)	O^{iii}—Cr—Sr^{xii}	125.3
O^{x}—Sr—O^{xi}	178.75 (16)	O^{xviii}—Cr—Sr^{xii}	54.7
Ni′—O—Os	0.0	O^{v}—Cr—Sr^{xii}	125.3
Ni′—O—Ni"	180.0	O^{xix}—Cr—Sr^{xii}	125.3
Os—O—Ni"	180.0	O—Cr—Sr^{xii}	54.7
Ni′—O—Os′	180.0	Sr—Cr—Sr^{xii}	109.5
Os—O—Os′	180.0	Sr^{xix}—Cr—Sr^{xii}	70.5
Ni"—O—Os′	0.0	Sr^{xi}—Cr—Sr^{xii}	70.5
Ni′—O—Cr	180.0	Sr^{xx}—Cr—Sr^{xii}	180.0
Os—O—Cr	180.0	O^{xvii}—Cr—Sr^{xxi}	125.3
Ni"—O—Cr	0.0	O^{iii}—Cr—Sr^{xxi}	54.7
Os′—O—Cr	0.0	O^{xviii}—Cr—Sr^{xxi}	54.7
Ni′—O—Sr^{xii}	90.63 (8)	O^{v}—Cr—Sr^{xxi}	125.3
Os—O—Sr^{xii}	90.63 (8)	O^{xix}—Cr—Sr^{xxi}	54.7
Ni"—O—Sr^{xii}	89.37 (8)	O—Cr—Sr^{xxi}	125.3
Os′—O—Sr^{xii}	89.37 (8)	Sr—Cr—Sr^{xxi}	109.5
Cr—O—Sr^{xii}	89.37 (8)	Sr^{xix}—Cr—Sr^{xxi}	70.5
Ni′—O—Sr	90.63 (8)	Sr^{xi}—Cr—Sr^{xxi}	70.5
Os—O—Sr	90.63 (8)	Sr^{xx}—Cr—Sr^{xxi}	70.5
Ni"—O—Sr	89.37 (8)	Sr^{xii}—Cr—Sr^{xxi}	109.5
Os′—O—Sr	89.37 (8)	O^{xvii}—Os′—O^{iii}	180.0
Cr—O—Sr	89.37 (8)	O^{xvii}—Os′—O^{xviii}	90.000 (1)
Sr^{xii}—O—Sr	178.75 (16)	O^{iii}—Os′—O^{xviii}	90.0
Ni′—O—Sr^{x}	90.63 (8)	O^{xvii}—Os′—O^{v}	90.0
Os—O—Sr^{x}	90.63 (8)	O^{iii}—Os′—O^{v}	90.000 (1)
Ni"—O—Sr^{x}	89.37 (8)	O^{xviii}—Os′—O^{v}	180.0
Os′—O—Sr^{x}	89.37 (8)	O^{xvii}—Os′—O^{xix}	90.0
Cr—O—Sr^{x}	89.37 (8)	O^{iii}—Os′—O^{xix}	90.0
Sr^{xii}—O—Sr^{x}	89.993 (2)	O^{xviii}—Os′—O^{xix}	90.0
Sr—O—Sr^{x}	89.993 (2)	O^{v}—Os′—O^{xix}	90.0
Ni′—O—Sr^{xi}	90.63 (8)	O^{xvii}—Os′—O	90.0
Os—O—Sr^{xi}	90.63 (8)	O^{iii}—Os′—O	90.0
Ni"—O—Sr^{xi}	89.37 (8)	O^{xviii}—Os′—O	90.0
Os′—O—Sr^{xi}	89.37 (8)	O^{v}—Os′—O	90.0
Cr—O—Sr^{xi}	89.37 (8)	O^{xix}—Os′—O	180.0
Sr^{xii}—O—Sr^{xi}	89.993 (2)	O^{xvii}—Os′—Sr	125.3
Sr—O—Sr^{xi}	89.993 (2)	O^{iii}—Os′—Sr	54.7
Sr^{x}—O—Sr^{xi}	178.75 (16)	O^{xviii}—Os′—Sr	125.3
O—Os—O^{vii}	90.0	O^{v}—Os′—Sr	54.7
O—Os—O^{xiii}	90.0	O^{xix}—Os′—Sr	125.3

O^{vii}—Os—O^{xiii}	180.0	O—Os′—Sr	54.7
O—Os—O^{ix}	90.0	O^{xvii}—Os′—Sr^{xix}	54.7
O^{vii}—Os—O^{ix}	90.0	O^{iii}—Os′—Sr^{xix}	125.3
O^{xiii}—Os—O^{ix}	90.0	O^{xviii}—Os′—Sr^{xix}	54.7
O—Os—O^{xiv}	90.0	O^{v}—Os′—Sr^{xix}	125.3
O^{vii}—Os—O^{xiv}	90.0	O^{xix}—Os′—Sr^{xix}	54.7
O^{xiii}—Os—O^{xiv}	90.0	O—Os′—Sr^{xix}	125.3
O^{ix}—Os—O^{xiv}	180.0	Sr—Os′—Sr^{xix}	180.0
O—Os—O^{xv}	180.0	O^{xvii}—Os′—Sr^{xi}	125.3
O^{vii}—Os—O^{xv}	90.0	O^{iii}—Os′—Sr^{xi}	54.7
O^{xiii}—Os—O^{xv}	90.0	O^{xviii}—Os′—Sr^{xi}	54.7
O^{ix}—Os—O^{xv}	90.0	O^{v}—Os′—Sr^{xi}	125.3
O^{xiv}—Os—O^{xv}	90.0	O^{xix}—Os′—Sr^{xi}	125.264 (1)
O—Os—Sr^{xii}	54.7	O—Os′—Sr^{xi}	54.7
O^{vii}—Os—Sr^{xii}	125.3	Sr—Os′—Sr^{xi}	70.5
O^{xiii}—Os—Sr^{xii}	54.7	Sr^{xix}—Os′—Sr^{xi}	109.5
O^{ix}—Os—Sr^{xii}	125.3	O^{xvii}—Os′—Sr^{xx}	125.3
O^{xiv}—Os—Sr^{xii}	54.7	O^{iii}—Os′—Sr^{xx}	54.7
O^{xv}—Os—Sr^{xii}	125.3	O^{xviii}—Os′—Sr^{xx}	125.264 (1)
O—Os—Sr^{xvi}	125.3	O^{v}—Os′—Sr^{xx}	54.7
O^{vii}—Os—Sr^{xvi}	54.7	O^{xix}—Os′—Sr^{xx}	54.7
O^{xiii}—Os—Sr^{xvi}	125.3	O—Os′—Sr^{xx}	125.3
O^{ix}—Os—Sr^{xvi}	54.7	Sr—Os′—Sr^{xx}	70.5
O^{xiv}—Os—Sr^{xvi}	125.3	Sr^{xix}—Os′—Sr^{xx}	109.5
O^{xv}—Os—Sr^{xvi}	54.7	Sr^{xi}—Os′—Sr^{xx}	109.5
Sr^{xii}—Os—Sr^{xvi}	180.0	O^{xvii}—Os′—Sr^{xii}	54.7
O—Os—Sr	54.7	O^{iii}—Os′—Sr^{xii}	125.3
O^{vii}—Os—Sr	54.7	O^{xviii}—Os′—Sr^{xii}	54.7
O^{xiii}—Os—Sr	125.3	O^{v}—Os′—Sr^{xii}	125.3
O^{ix}—Os—Sr	54.7	O^{xix}—Os′—Sr^{xii}	125.3
O^{xiv}—Os—Sr	125.3	O—Os′—Sr^{xii}	54.7
O^{xv}—Os—Sr	125.3	Sr—Os′—Sr^{xii}	109.5
Sr^{xii}—Os—Sr	109.5	Sr^{xix}—Os′—Sr^{xii}	70.5
Sr^{xvi}—Os—Sr	70.5	Sr^{xi}—Os′—Sr^{xii}	70.5
O—Os—Sr^{x}	54.7	Sr^{xx}—Os′—Sr^{xii}	180.0
O^{vii}—Os—Sr^{x}	125.3	O^{xvii}—Os′—Sr^{xxi}	125.3
O^{xiii}—Os—Sr^{x}	54.7	O^{iii}—Os′—Sr^{xxi}	54.7
O^{ix}—Os—Sr^{x}	54.7	O^{xviii}—Os′—Sr^{xxi}	54.7
O^{xiv}—Os—Sr^{x}	125.3	O^{v}—Os′—Sr^{xxi}	125.3
O^{xv}—Os—Sr^{x}	125.3	O^{xix}—Os′—Sr^{xxi}	54.7
Sr^{xii}—Os—Sr^{x}	70.5	O—Os′—Sr^{xxi}	125.3
Sr^{xvi}—Os—Sr^{x}	109.5	Sr—Os′—Sr^{xxi}	109.5
Sr—Os—Sr^{x}	70.5	Sr^{xix}—Os′—Sr^{xxi}	70.5
O—Os—Sr^{xv}	125.3	Sr^{xi}—Os′—Sr^{xxi}	70.5
O^{vii}—Os—Sr^{xv}	125.3	Sr^{xx}—Os′—Sr^{xxi}	70.5
O^{xiii}—Os—Sr^{xv}	54.7	Sr^{xii}—Os′—Sr^{xxi}	109.5
O^{ix}—Os—Sr^{xv}	125.3	O^{xvii}—Ni"—O^{iii}	180.0
O^{xiv}—Os—Sr^{xv}	54.7	O^{xvii}—Ni"—O^{xviii}	90.000 (1)

O^{xv}—Os—Sr^{xv}	54.7	O^{iii}—Ni"—O^{xviii}	90.0
Sr^{xii}—Os—Sr^{xv}	70.5	O^{xvii}—Ni"—O^{v}	90.0
Sr^{xvi}—Os—Sr^{xv}	109.5	O^{iii}—Ni"—O^{v}	90.000 (1)
Sr—Os—Sr^{xv}	180.0	O^{xviii}—Ni"—O^{v}	180.0
Sr^{x}—Os—Sr^{xv}	109.5	O^{xvii}—Ni"—O^{xix}	90.0
O—Os—Sr^{xi}	54.7	O^{iii}—Ni"—O^{xix}	90.0
O^{vii}—Os—Sr^{xi}	54.7	O^{xviii}—Ni"—O^{xix}	90.0
O^{xiii}—Os—Sr^{xi}	125.3	O^{v}—Ni"—O^{xix}	90.0
O^{ix}—Os—Sr^{xi}	125.3	O^{xvii}—Ni"—O	90.0
O^{xiv}—Os—Sr^{xi}	54.7	O^{iii}—Ni"—O	90.0
O^{xv}—Os—Sr^{xi}	125.3	O^{xviii}—Ni"—O	90.0
Sr^{xii}—Os—Sr^{xi}	70.5	O^{v}—Ni"—O	90.0
Sr^{xvi}—Os—Sr^{xi}	109.5	O^{xix}—Ni"—O	180.0
Sr—Os—Sr^{xi}	70.5	O^{xvii}—Ni"—Sr	125.3
Sr^{x}—Os—Sr^{xi}	109.5	O^{iii}—Ni"—Sr	54.7
Sr^{xv}—Os—Sr^{xi}	109.5	O^{xviii}—Ni"—Sr	125.3
O—Ni′—O^{vii}	90.0	O^{v}—Ni"—Sr	54.7
O—Ni′—O^{xiii}	90.0	O^{xix}—Ni"—Sr	125.3
O^{vii}—Ni′—O^{xiii}	180.0	O—Ni"—Sr	54.7
O—Ni′—O^{ix}	90.0	O^{xvii}—Ni"—Sr^{xix}	54.7
O^{vii}—Ni′—O^{ix}	90.0	O^{iii}—Ni"—Sr^{xix}	125.3
O^{xiii}—Ni′—O^{ix}	90.0	O^{xviii}—Ni"—Sr^{xix}	54.7
O—Ni′—O^{xiv}	90.0	O^{v}—Ni"—Sr^{xix}	125.3
O^{vii}—Ni′—O^{xiv}	90.0	O^{xix}—Ni"—Sr^{xix}	54.7
O^{xiii}—Ni′—O^{xiv}	90.0	O—Ni"—Sr^{xix}	125.3
O^{ix}—Ni′—O^{xiv}	180.0	Sr—Ni"—Sr^{xix}	180.0
O—Ni′—O^{xv}	180.0	O^{xvii}—Ni"—Sr^{xi}	125.3
O^{vii}—Ni′—O^{xv}	90.0	O^{iii}—Ni"—Sr^{xi}	54.7
O^{xiii}—Ni′—O^{xv}	90.0	O^{xviii}—Ni"—Sr^{xi}	54.7
O^{ix}—Ni′—O^{xv}	90.0	O^{v}—Ni"—Sr^{xi}	125.3
O^{xiv}—Ni′—O^{xv}	90.0	O^{xix}—Ni"—Sr^{xi}	125.264 (1)
O—Ni′—Sr^{xii}	54.7	O—Ni"—Sr^{xi}	54.7
O^{vii}—Ni′—Sr^{xii}	125.3	Sr—Ni"—Sr^{xi}	70.5
O^{xiii}—Ni′—Sr^{xii}	54.7	Sr^{xix}—Ni"—Sr^{xi}	109.5
O^{ix}—Ni′—Sr^{xii}	125.3	O^{xvii}—Ni"—Sr^{xx}	125.3
O^{xiv}—Ni′—Sr^{xii}	54.7	O^{iii}—Ni"—Sr^{xx}	54.7
O^{xv}—Ni′—Sr^{xii}	125.3	O^{xviii}—Ni"—Sr^{xx}	125.264 (1)
O—Ni′—Sr^{xvi}	125.3	O^{v}—Ni"—Sr^{xx}	54.7
O^{vii}—Ni′—Sr^{xvi}	54.7	O^{xix}—Ni"—Sr^{xx}	54.7
O^{xiii}—Ni′—Sr^{xvi}	125.3	O—Ni"—Sr^{xx}	125.3
O^{ix}—Ni′—Sr^{xvi}	54.7	Sr—Ni"—Sr^{xx}	70.5
O^{xiv}—Ni′—Sr^{xvi}	125.3	Sr^{xix}—Ni"—Sr^{xx}	109.5
O^{xv}—Ni′—Sr^{xvi}	54.7	Sr^{xi}—Ni"—Sr^{xx}	109.5
Sr^{xii}—Ni′—Sr^{xvi}	180.0	O^{xvii}—Ni"—Sr^{xii}	54.7
O—Ni′—Sr	54.7	O^{iii}—Ni"—Sr^{xii}	125.3
O^{vii}—Ni′—Sr	54.7	O^{xviii}—Ni"—Sr^{xii}	54.7
O^{xiii}—Ni′—Sr	125.3	O^{v}—Ni"—Sr^{xii}	125.3
O^{ix}—Ni′—Sr	54.7	O^{xix}—Ni"—Sr^{xii}	125.3

O^{xiv}—Ni′—Sr	125.3	O—Ni"—Sr^{xii}	54.7
O^{xv}—Ni′—Sr	125.3	Sr—Ni"—Sr^{xii}	109.5
Sr^{xii}—Ni′—Sr	109.5	Sr^{xix}—Ni"—Sr^{xii}	70.5
Sr^{xvi}—Ni′—Sr	70.5	Sr^{xi}—Ni"—Sr^{xii}	70.5
O—Ni′—Sr^{x}	54.7	Sr^{xx}—Ni"—Sr^{xii}	180.0
O^{vii}—Ni′—Sr^{x}	125.3	O^{xvii}—Ni"—Sr^{xxi}	125.3
O^{xiii}—Ni′—Sr^{x}	54.7	O^{iii}—Ni"—Sr^{xxi}	54.7
O^{ix}—Ni′—Sr^{x}	54.7	O^{xviii}—Ni"—Sr^{xxi}	54.7
O^{xiv}—Ni′—Sr^{x}	125.3	O^{v}—Ni"—Sr^{xxi}	125.3
O^{xv}—Ni′—Sr^{x}	125.3	O^{xix}—Ni"—Sr^{xxi}	54.7
Sr^{xii}—Ni′—Sr^{x}	70.5	O—Ni"—Sr^{xxi}	125.3
Sr^{xvi}—Ni′—Sr^{x}	109.5	Sr—Ni"—Sr^{xxi}	109.5
Sr—Ni′—Sr^{x}	70.5	Sr^{xix}—Ni"—Sr^{xxi}	70.5
O—Ni′—Sr^{xv}	125.3	Sr^{xi}—Ni"—Sr^{xxi}	70.5
O^{vii}—Ni′—Sr^{xv}	125.3	Sr^{xx}—Ni"—Sr^{xxi}	70.5
O^{xiii}—Ni′—Sr^{xv}	54.7	Sr^{xii}—Ni"—Sr^{xxi}	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) −*x*+1/2, −*y*+1, −*z*+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.