



Redetermination of Sr₂PdO₃ from single-crystal X-ray data

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The crystal structure redetermination of Sr₂PdO₃ (distrontium palladium trioxide) was carried out using high-quality single-crystal X-ray data. The Sr₂PdO₃ structure has been described previously in at least three reports [Wasel-Nielen & Hoppe (1970). *Z. Anorg. Allg. Chem.* **375**, 209–213; Muller & Roy (1971). *Adv. Chem. Ser.* **98**, 28–38; Nagata *et al.* (2002). *J. Alloys Compd.* **346**, 50–56], all based on powder X-ray diffraction data. The current structure refinement of Sr₂PdO₃, as compared to previous powder data refinements, leads to more precise cell parameters and fractional coordinates, together with anisotropic displacement parameters for all sites. The compound is confirmed to have the orthorhombic Sr₂CuO₃ structure type (space group *Immm*) as reported previously. The structure consists of infinite chains of corner-sharing PdO₄ plaquettes interspersed by Sr^{II} atoms. A brief comparison of Sr₂PdO₃ with the related K₂NiF₄ structure type is given.

1. Chemical context

Low-dimensional transition-metal oxides with chain structures have received attention since they can enable interesting physical phenomena such as spin 1/2 antiferromagnetic Heisenberg coupling (Motoyama *et al.*, 1996; Takigawa *et al.*, 1996), superconductivity (Hiroi *et al.*, 1993), ultrafast non-linear optical response (Ogasawara *et al.*, 2000) or even glucose sensing (El-Ads *et al.*, 2016). The particularly relevant sub-family based on square-planar MO₄ (*M* = divalent metal) primary building units is dominated by oxidocuprates(II), while the chemistry of respective palladates(II), showing the same preference for a square-planar coordination by oxygen, is much less explored.

Here we address Sr₂PdO₃, which has previously been obtained as a microcrystalline material (Wasel-Nielen & Hoppe, 1970; Muller & Roy, 1971; Nagata *et al.*, 2002). Based on evaluations of powder X-ray diffractograms, Sr₂PdO₃ was identified as being isostructural with Sr₂CuO₃ (Teske & Müller-Buschbaum, 1969; Weller & Lines, 1989) and Sr₂FeO₃ (Tassel *et al.*, 2013). However, structural details derived from the given atomic parameters have only been reported with large uncertainties (Muller & Roy, 1971; Nagata *et al.*, 2002). Therefore, a redetermination of Sr₂PdO₃ based on single crystal X-ray data seemed appropriate.

2. Structural commentary

The crystal structure of Sr₂PdO₃ is essentially the same as determined previously (Wasel-Nielen & Hoppe, 1970; Muller

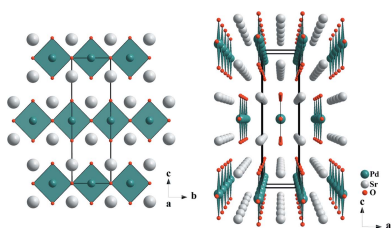


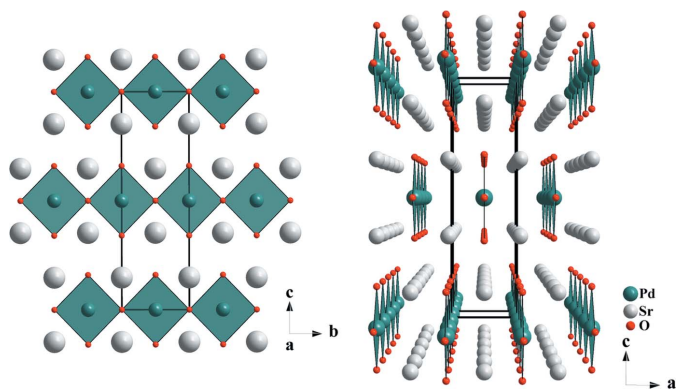
Table 1

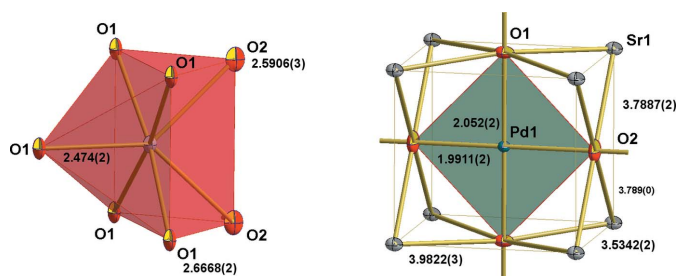
 Comparison of lattice parameters and bond lengths (Å) in Sr₂PdO₃ determined in different studies.

	1970 work ^a	1971 work ^b	2002 work ^c	This work
<i>a</i>	3.977	3.97	3.985	3.5342 (2)
<i>b</i>	3.53	3.544	3.539	3.9822 (3)
<i>c</i>	12.82	12.84	12.847	12.8414 (8)
Pd—O1 (×2)	2.08	2.045	2.068	2.052 (2)
Pd—O2 (×2)	1.99	1.985	1.993	1.9911 (1)
Sr—O1	2.45	2.504	2.467	2.474 (2)
Sr—O1 (×4)	2.67	2.668	2.671	2.6668 (2)
Sr—O2 (×2)	2.58	2.57	2.588	2.5906 (3)

 References: (a) Wasel-Nielen & Hoppe (1970); (b) Muller & Roy (1971); (c) Nagata *et al.* (2002).

& Roy, 1971; Nagata *et al.*, 2002). The lattice parameters (Table 1) are almost identical to those in the previous reports but with higher precision. The Pd^{II} atom occupies the 2*d* crystallographic sites with *mmm* site symmetry. We would like to point out that we chose a different cell setting as compared to all the previous reports, where the Pd^{II} atom was chosen to be located at the cell origin (site 2*a*; 0, 0, 0; hence the different site designations). The Pd^{II} atom forms distorted PdO₄ square planes, which are linked by sharing oxygen atoms in the *trans*-position to form infinite chains extending along the *b*-axis direction as shown in Fig. 1. Corresponding to this connectivity pattern, the Pd—O bond lengths are longer for the shared oxygen atoms, 2.052 (2) Å, and shorter for the terminal ones, 1.9911 (2) Å. The Sr atom is situated at the 4*j* Wyckoff site having *mm2* site symmetry. It is seven-coordinate in a monocapped trigonal-prismatic fashion by oxygen with three different bond lengths (Table 1, Fig. 2). In addition to the square-planar first coordination of Pd^{II} with oxygen, the second consists of eight Sr^{II} atoms present at the corner of a cuboid with dimension 3.5342 (2) × 3.7887 (2) × 3.9822 (3) Å³ (Fig. 2). Of the two kinds of oxygen atoms, both surrounded by six metal ions that form distorted octahedra, O1 is coordinated by one Pd^{II} atom [2.052 (2) Å] and five Sr^{II} atoms with one short [2.474 (2) Å] and four long distances [2.6668 (2) Å] (Fig. 3). O2 is connected to four equidistant Sr^{II} [2.5906 (3) Å] and two Pd^{II} atoms [1.9911 (2) Å] (Fig. 3). In our current


Figure 1

 Crystal structure of Sr₂PdO₃ viewed along the *a* axis (left) and along the *b* axis (right).

Figure 2

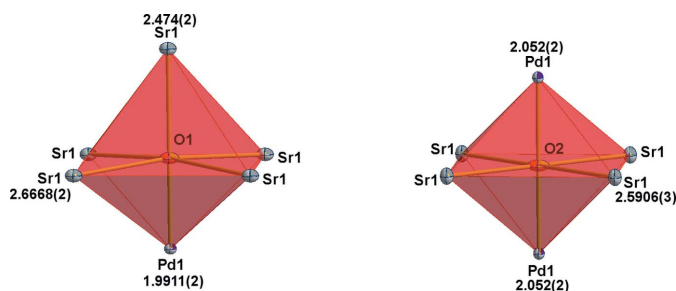
 Coordination around the Sr^{II} (left) and Pd^{II} atoms (right). All atoms are drawn with displacement ellipsoids at the 80% probability level. Distances are in Å.

structure determination, much more precise values of the cell parameters along with the *z* parameters of Sr and O1 have been determined, consequently, yielding very precise values for the bond lengths (see Table 1). The quality of the current refinement is also clearly reflected by better reliability factors (see Table 2) as compared to the previous refinements. The atomic arrangement described here is same as provided by Wasel-Nielen & Hoppe (1970).

The structural features discussed above are closely related to those of the K₂NiF₄ type of structure, which is regarded as the prototype structure for all the high *T_c* cuprates. K₂NiF₄ consists of layers of corner-shared NiF₆ octahedra extending in the *ab* plane. One can derive the Sr₂PdO₃ structure from the K₂NiF₄ structure by systematically removing the bridging F atoms from the NiF₆ octahedra lying in the *a*-axis direction (Fig. 4). This would reduce the dimensionality of the layer, resulting in linear chains of square planes connected by edges along only one direction.

3. Synthesis and crystallization

Millimeter-sized block-shaped crystals of dark-yellow colour with composition Sr₂PdO₃ as confirmed by SEM–EDS, were obtained from a mixture of different phases while attempting to synthesize SrPd₃O₄ using a KOH flux (Smallwood *et al.*, 2000). SrCO₃ and Pd metal powder were mixed in the molar ratio of 2:3, placed in an alumina crucible, and 15 grams of KOH pellets were added on top. The crucible was heated in a muffle furnace to 1023 K in 24 h with a 6 h dwell time. The


Figure 3

Coordination polyhedra of two types of oxygen atoms, O1 (left) and O2 (right). All atoms are drawn with displacement ellipsoids at the 80% probability level. Distances are in Å.

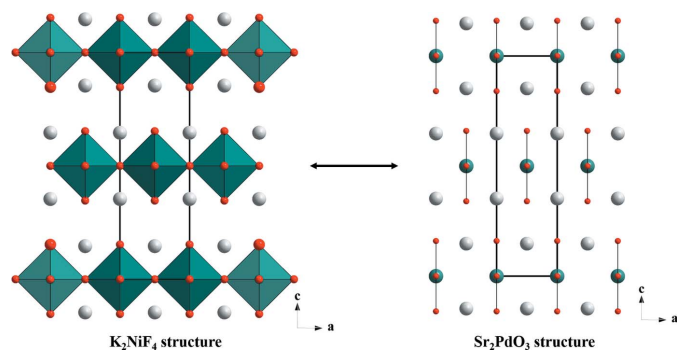


Figure 4
Interconversion of the Sr_2PdO_3 and K_2NiF_4 structures.

furnace was then cooled slowly to 873 K over 125 h after which it was switched off and allowed to cool naturally. The product was washed several times with water to remove the solidified flux and subsequently rinsed with ethanol.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 El-Ads, E. H., Galal, A. & Atta, N. F. (2016). *RSC Adv.* **6**, 16183–16196.
 Hiroi, Z., Takano, M., Azuma, M. & Takeda, Y. (1993). *Nature*, **364**, 315–317.
 Motoyama, N., Eisaki, H. & Uchida, S. (1996). *Phys. Rev. Lett.* **76**, 3212–3215.
 Muller, O. & Roy, R. (1971). *Adv. Chem. Ser.* **98**, 28–38.
 Nagata, Y., Taniguchi, T., Tanaka, G., Satho, M. & Samata, H. (2002). *J. Alloys Compd.* **346**, 50–56.
 Ogasawara, T., Ashida, M., Motoyama, N., Eisaki, H., Uchida, S., Tokura, Y., Ghosh, H., Shukla, A., Mazumdar, S. & Kuwata-Gonokami, M. (2000). *Phys. Rev. Lett.* **85**, 2204–2207.

Table 2
Experimental details.

Crystal data	Sr_2PdO_3
Chemical formula	329.64
M_r	Orthorhombic, <i>Immm</i>
Crystal system, space group	296
Temperature (K)	3.5342 (2), 3.9822 (3), 12.8414 (8)
a, b, c (Å)	180.73 (2)
V (Å ³)	2
Z	Mo $K\alpha$
Radiation type	34.15
μ (mm ⁻¹)	0.18 × 0.16 × 0.12
Crystal size (mm)	
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2009)
T_{\min}, T_{\max}	0.062, 0.102
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8304, 178, 176
R_{int}	0.035
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.009, 0.021, 1.27
No. of reflections	178
No. of parameters	16
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.43, -0.51

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006).

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
 Smallwood, P. L., Smith, M. D. & zur Loye, H. C. (2000). *J. Cryst. Growth*, **216**, 299–303.
 Takigawa, M., Motoyama, N., Eisaki, H. & Uchida, S. (1996). *Phys. Rev. Lett.* **76**, 4612–4615.
 Tassel, C., Seinberg, L., Hayashi, N., Ganesanpotti, S., Ajiro, Y., Kobayashi, Y. & Kageyama, H. (2013). *Inorg. Chem.* **52**, 6096–6102.
 Teske, C. L. & Müller-Buschbaum, Hk. (1969). *Z. Anorg. Allg. Chem.* **371**, 325–332.
 Wasel-Nielsen, H. D. & Hoppe, R. (1970). *Z. Anorg. Allg. Chem.* **375**, 209–213.
 Weller, M. T. & Lines, D. R. (1989). *J. Solid State Chem.* **82**, 21–29.

supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Distrontium palladium trioxide

Crystal data

Sr ₂ PdO ₃	$D_x = 6.057 \text{ Mg m}^{-3}$
$M_r = 329.64$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, <i>Immm</i>	Cell parameters from 1490 reflections
$a = 3.5342 (2) \text{ \AA}$	$\theta = 3.2\text{--}29.9^\circ$
$b = 3.9822 (3) \text{ \AA}$	$\mu = 34.15 \text{ mm}^{-1}$
$c = 12.8414 (8) \text{ \AA}$	$T = 296 \text{ K}$
$V = 180.73 (2) \text{ \AA}^3$	Block, yellow-brown
$Z = 2$	$0.18 \times 0.16 \times 0.12 \text{ mm}$
$F(000) = 292$	

Data collection

Bruker APEXII CCD diffractometer	178 independent reflections
φ and ω scans	176 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2009)	$R_{\text{int}} = 0.035$
$T_{\text{min}} = 0.062$, $T_{\text{max}} = 0.102$	$\theta_{\text{max}} = 29.9^\circ$, $\theta_{\text{min}} = 3.2^\circ$
8304 measured reflections	$h = -4 \rightarrow 4$
	$k = -5 \rightarrow 5$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0092P)^2 + 0.2817P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.009$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$wR(F^2) = 0.021$	$\Delta\rho_{\text{max}} = 0.43 \text{ e \AA}^{-3}$
$S = 1.27$	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$
178 reflections	Extinction correction: <i>SHELXL-2014/7</i>
16 parameters	(Sheldrick, 2015),
0 restraints	$Fc^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0059 (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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd1	0.5000	0.0000	0.5000	0.00493 (11)
Sr1	0.5000	0.0000	0.14752 (2)	0.00656 (11)
O1	0.5000	0.0000	0.34021 (18)	0.0085 (5)
O2	0.5000	0.5000	0.5000	0.0128 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.00765 (19)	0.00396 (17)	0.00320 (18)	0.000	0.000	0.000
Sr1	0.00752 (17)	0.00760 (16)	0.00456 (17)	0.000	0.000	0.000
O1	0.0117 (13)	0.0101 (12)	0.0037 (11)	0.000	0.000	0.000
O2	0.021 (2)	0.0035 (15)	0.0134 (18)	0.000	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Pd1—O2 ⁱ	1.9911 (1)	Sr1—O1 ^{ix}	2.6668 (2)
Pd1—O2	1.9911 (1)	Sr1—O1 ^{vii}	2.6668 (2)
Pd1—O1	2.052 (2)	Sr1—Pd1 ^{xi}	3.2674 (2)
Pd1—O1 ⁱⁱ	2.052 (2)	Sr1—Pd1 ^{xii}	3.2674 (2)
Pd1—Sr1 ⁱⁱⁱ	3.2674 (2)	Sr1—Pd1 ^{xiii}	3.2674 (2)
Pd1—Sr1 ^{iv}	3.2674 (2)	Sr1—Pd1 ^{xiv}	3.2674 (2)
Pd1—Sr1 ^v	3.2674 (2)	Sr1—Sr1 ^{xv}	3.5342 (2)
Pd1—Sr1 ^{vi}	3.2674 (2)	O1—Sr1 ^{viii}	2.6668 (2)
Pd1—Sr1 ^{vii}	3.2674 (2)	O1—Sr1 ⁱⁱⁱ	2.6668 (2)
Pd1—Sr1 ^{viii}	3.2674 (2)	O1—Sr1 ^{vii}	2.6668 (2)
Pd1—Sr1 ^{ix}	3.2674 (2)	O1—Sr1 ^{ix}	2.6668 (2)
Pd1—Sr1 ^x	3.2674 (2)	O2—Pd1 ^{xvi}	1.9911 (1)
Sr1—O1	2.474 (2)	O2—Sr1 ^{ix}	2.5906 (3)
Sr1—O2 ^{xi}	2.5906 (3)	O2—Sr1 ^{iv}	2.5906 (3)
Sr1—O2 ^{xii}	2.5906 (3)	O2—Sr1 ^{viii}	2.5906 (3)
Sr1—O1 ^{viii}	2.6668 (2)	O2—Sr1 ^{vi}	2.5906 (3)
Sr1—O1 ⁱⁱⁱ	2.6668 (2)		
O2 ⁱ —Pd1—O2	180.0	O1—Sr1—O1 ^{vii}	86.61 (5)
O2 ⁱ —Pd1—O1	90.0	O2 ^{xi} —Sr1—O1 ^{vii}	119.68 (4)
O2—Pd1—O1	90.0	O2 ^{xii} —Sr1—O1 ^{vii}	65.87 (4)
O2 ⁱ —Pd1—O1 ⁱⁱ	90.0	O1 ^{viii} —Sr1—O1 ^{vii}	96.597 (9)
O2—Pd1—O1 ⁱⁱ	90.0	O1 ⁱⁱⁱ —Sr1—O1 ^{vii}	83.000 (8)
O1—Pd1—O1 ⁱⁱ	180.0	O1 ^{ix} —Sr1—O1 ^{vii}	173.22 (10)

O2 ⁱ —Pd1—Sr1 ⁱⁱⁱ	52.455 (3)	O1—Sr1—Pd1 ^{xi}	125.435 (5)
O2—Pd1—Sr1 ⁱⁱⁱ	127.545 (3)	O2 ^{xi} —Sr1—Pd1 ^{xi}	37.546 (3)
O1—Pd1—Sr1 ⁱⁱⁱ	54.565 (5)	O2 ^{xii} —Sr1—Pd1 ^{xi}	86.845 (8)
O1 ⁱⁱ —Pd1—Sr1 ⁱⁱⁱ	125.435 (5)	O1 ^{viii} —Sr1—Pd1 ^{xi}	147.95 (5)
O2 ⁱ —Pd1—Sr1 ^{iv}	127.545 (3)	O1 ⁱⁱⁱ —Sr1—Pd1 ^{xi}	38.82 (5)
O2—Pd1—Sr1 ^{iv}	52.455 (3)	O1 ^{ix} —Sr1—Pd1 ^{xi}	97.52 (3)
O1—Pd1—Sr1 ^{iv}	125.435 (5)	O1 ^{vii} —Sr1—Pd1 ^{xi}	86.43 (3)
O1 ⁱⁱ —Pd1—Sr1 ^{iv}	54.565 (5)	O1—Sr1—Pd1 ^{xii}	125.435 (5)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^{iv}	180.0	O2 ^{xi} —Sr1—Pd1 ^{xii}	86.845 (8)
O2 ⁱ —Pd1—Sr1 ^v	52.455 (4)	O2 ^{xii} —Sr1—Pd1 ^{xii}	37.546 (3)
O2—Pd1—Sr1 ^v	127.545 (3)	O1 ^{viii} —Sr1—Pd1 ^{xii}	97.52 (3)
O1—Pd1—Sr1 ^v	125.435 (5)	O1 ⁱⁱⁱ —Sr1—Pd1 ^{xii}	86.43 (3)
O1 ⁱⁱ —Pd1—Sr1 ^v	54.565 (5)	O1 ^{ix} —Sr1—Pd1 ^{xii}	147.95 (5)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^v	70.871 (10)	O1 ^{vii} —Sr1—Pd1 ^{xii}	38.82 (5)
Sr1 ^{iv} —Pd1—Sr1 ^v	109.129 (10)	Pd1 ^{xi} —Sr1—Pd1 ^{xii}	65.481 (6)
O2 ⁱ —Pd1—Sr1 ^{vi}	127.545 (3)	O1—Sr1—Pd1 ^{xiii}	125.435 (5)
O2—Pd1—Sr1 ^{vi}	52.455 (4)	O2 ^{xi} —Sr1—Pd1 ^{xiii}	86.845 (9)
O1—Pd1—Sr1 ^{vi}	125.435 (5)	O2 ^{xii} —Sr1—Pd1 ^{xiii}	37.546 (3)
O1 ⁱⁱ —Pd1—Sr1 ^{vi}	54.565 (5)	O1 ^{viii} —Sr1—Pd1 ^{xiii}	38.82 (5)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^{vi}	114.520 (6)	O1 ⁱⁱⁱ —Sr1—Pd1 ^{xiii}	147.95 (5)
Sr1 ^{iv} —Pd1—Sr1 ^{vi}	65.480 (6)	O1 ^{ix} —Sr1—Pd1 ^{xiii}	86.43 (3)
Sr1 ^v —Pd1—Sr1 ^{vi}	75.090 (7)	O1 ^{vii} —Sr1—Pd1 ^{xiii}	97.52 (3)
O2 ⁱ —Pd1—Sr1 ^{vii}	52.455 (3)	Pd1 ^{xi} —Sr1—Pd1 ^{xiii}	109.130 (10)
O2—Pd1—Sr1 ^{vii}	127.545 (3)	Pd1 ^{xii} —Sr1—Pd1 ^{xiii}	75.091 (7)
O1—Pd1—Sr1 ^{vii}	54.565 (5)	O1—Sr1—Pd1 ^{xiv}	125.435 (5)
O1 ⁱⁱ —Pd1—Sr1 ^{vii}	125.435 (5)	O2 ^{xi} —Sr1—Pd1 ^{xiv}	37.546 (3)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^{vii}	65.480 (5)	O2 ^{xii} —Sr1—Pd1 ^{xiv}	86.845 (8)
Sr1 ^{iv} —Pd1—Sr1 ^{vii}	114.520 (6)	O1 ^{viii} —Sr1—Pd1 ^{xiv}	86.43 (3)
Sr1 ^v —Pd1—Sr1 ^{vii}	104.910 (7)	O1 ⁱⁱⁱ —Sr1—Pd1 ^{xiv}	97.52 (3)
Sr1 ^{vi} —Pd1—Sr1 ^{vii}	180.0	O1 ^{ix} —Sr1—Pd1 ^{xiv}	38.82 (5)
O2 ⁱ —Pd1—Sr1 ^{viii}	127.545 (3)	O1 ^{vii} —Sr1—Pd1 ^{xiv}	147.95 (5)
O2—Pd1—Sr1 ^{viii}	52.455 (3)	Pd1 ^{xi} —Sr1—Pd1 ^{xiv}	75.091 (7)
O1—Pd1—Sr1 ^{viii}	54.565 (5)	Pd1 ^{xii} —Sr1—Pd1 ^{xiv}	109.130 (10)
O1 ⁱⁱ —Pd1—Sr1 ^{viii}	125.435 (5)	Pd1 ^{xiii} —Sr1—Pd1 ^{xiv}	65.481 (6)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^{viii}	109.129 (10)	O1—Sr1—Sr1 ^{xv}	90.0
Sr1 ^{iv} —Pd1—Sr1 ^{viii}	70.871 (10)	O2 ^{xi} —Sr1—Sr1 ^{xv}	133.011 (5)
Sr1 ^v —Pd1—Sr1 ^{viii}	180.0	O2 ^{xii} —Sr1—Sr1 ^{xv}	46.991 (5)
Sr1 ^{vi} —Pd1—Sr1 ^{viii}	104.910 (7)	O1 ^{viii} —Sr1—Sr1 ^{xv}	48.500 (3)
Sr1 ^{vii} —Pd1—Sr1 ^{viii}	75.090 (7)	O1 ⁱⁱⁱ —Sr1—Sr1 ^{xv}	131.500 (4)
O2 ⁱ —Pd1—Sr1 ^{ix}	127.545 (4)	O1 ^{ix} —Sr1—Sr1 ^{xv}	131.500 (4)
O2—Pd1—Sr1 ^{ix}	52.455 (3)	O1 ^{vii} —Sr1—Sr1 ^{xv}	48.500 (4)
O1—Pd1—Sr1 ^{ix}	54.565 (5)	Pd1 ^{xi} —Sr1—Sr1 ^{xv}	122.741 (3)
O1 ⁱⁱ —Pd1—Sr1 ^{ix}	125.435 (5)	Pd1 ^{xii} —Sr1—Sr1 ^{xv}	57.260 (3)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^{ix}	75.090 (7)	Pd1 ^{xiii} —Sr1—Sr1 ^{xv}	57.260 (3)
Sr1 ^{iv} —Pd1—Sr1 ^{ix}	104.910 (7)	Pd1 ^{xiv} —Sr1—Sr1 ^{xv}	122.741 (3)
Sr1 ^v —Pd1—Sr1 ^{ix}	114.520 (6)	Pd1—O1—Sr1	180.0
Sr1 ^{vi} —Pd1—Sr1 ^{ix}	70.871 (10)	Pd1—O1—Sr1 ^{viii}	86.61 (5)
Sr1 ^{vii} —Pd1—Sr1 ^{ix}	109.129 (10)	Sr1—O1—Sr1 ^{viii}	93.39 (5)

Sr1 ^{viii} —Pd1—Sr1 ^{ix}	65.480 (6)	Pd1—O1—Sr1 ⁱⁱⁱ	86.61 (5)
O2 ⁱ —Pd1—Sr1 ^x	52.455 (3)	Sr1—O1—Sr1 ⁱⁱⁱ	93.39 (5)
O2—Pd1—Sr1 ^x	127.545 (3)	Sr1 ^{viii} —O1—Sr1 ⁱⁱⁱ	173.23 (10)
O1—Pd1—Sr1 ^x	125.435 (5)	Pd1—O1—Sr1 ^{vii}	86.61 (5)
O1 ⁱⁱ —Pd1—Sr1 ^x	54.565 (5)	Sr1—O1—Sr1 ^{vii}	93.39 (5)
Sr1 ⁱⁱⁱ —Pd1—Sr1 ^x	104.910 (7)	Sr1 ^{viii} —O1—Sr1 ^{vii}	96.597 (9)
Sr1 ^{iv} —Pd1—Sr1 ^x	75.090 (7)	Sr1 ⁱⁱⁱ —O1—Sr1 ^{vii}	83.001 (8)
Sr1 ^v —Pd1—Sr1 ^x	65.480 (5)	Pd1—O1—Sr1 ^{ix}	86.61 (5)
Sr1 ^{vi} —Pd1—Sr1 ^x	109.129 (10)	Sr1—O1—Sr1 ^{ix}	93.39 (5)
Sr1 ^{vii} —Pd1—Sr1 ^x	70.871 (10)	Sr1 ^{viii} —O1—Sr1 ^{ix}	83.001 (8)
Sr1 ^{viii} —Pd1—Sr1 ^x	114.520 (6)	Sr1 ⁱⁱⁱ —O1—Sr1 ^{ix}	96.597 (9)
Sr1 ^{ix} —Pd1—Sr1 ^x	180.0	Sr1 ^{vii} —O1—Sr1 ^{ix}	173.23 (10)
O1—Sr1—O2 ^{xi}	136.990 (5)	Pd1 ^{xvi} —O2—Pd1	180.0
O1—Sr1—O2 ^{xii}	136.990 (5)	Pd1 ^{xvi} —O2—Sr1 ^{ix}	90.0
O2 ^{xi} —Sr1—O2 ^{xii}	86.020 (11)	Pd1—O2—Sr1 ^{ix}	90.0
O1—Sr1—O1 ^{viii}	86.61 (5)	Pd1 ^{xvi} —O2—Sr1 ^{iv}	90.0
O2 ^{xi} —Sr1—O1 ^{viii}	119.68 (4)	Pd1—O2—Sr1 ^{iv}	90.0
O2 ^{xii} —Sr1—O1 ^{viii}	65.87 (4)	Sr1 ^{ix} —O2—Sr1 ^{iv}	180.0
O1—Sr1—O1 ⁱⁱⁱ	86.61 (5)	Pd1 ^{xvi} —O2—Sr1 ^{viii}	90.0
O2 ^{xi} —Sr1—O1 ⁱⁱⁱ	65.87 (4)	Pd1—O2—Sr1 ^{viii}	90.0
O2 ^{xii} —Sr1—O1 ⁱⁱⁱ	119.68 (4)	Sr1 ^{ix} —O2—Sr1 ^{viii}	86.018 (11)
O1 ^{viii} —Sr1—O1 ⁱⁱⁱ	173.22 (10)	Sr1 ^{iv} —O2—Sr1 ^{viii}	93.982 (11)
O1—Sr1—O1 ^{ix}	86.61 (5)	Pd1 ^{xvi} —O2—Sr1 ^{vi}	90.0
O2 ^{xi} —Sr1—O1 ^{ix}	65.87 (4)	Pd1—O2—Sr1 ^{vi}	90.0
O2 ^{xii} —Sr1—O1 ^{ix}	119.68 (4)	Sr1 ^{ix} —O2—Sr1 ^{vi}	93.982 (11)
O1 ^{viii} —Sr1—O1 ^{ix}	83.000 (8)	Sr1 ^{iv} —O2—Sr1 ^{vi}	86.018 (11)
O1 ⁱⁱⁱ —Sr1—O1 ^{ix}	96.597 (9)	Sr1 ^{viii} —O2—Sr1 ^{vi}	180.0

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