

Temperature-dependent structural behaviour of samarium cobalt oxide

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The crystal structure and thermal expansion of the perovskite samarium cobalt oxide (SmCoO_3) has been determined over the temperature range 295 to 1245 K by Rietveld analysis of X-ray powder diffraction data. Polycrystalline samples were prepared by a sol-gel synthesis route followed by high-temperature calcination in air. SmCoO_3 is orthorhombic ($Pnma$) at all temperatures and is isostructural with GdFeO_3 . The structure was refined as a distortion mode of a parent $Pm-3m$ structure. The thermal expansion was found to be non-linear and anisotropic, with maximum average linear thermal expansion coefficients of $34.0(3) \times 10^{-6} \text{ K}^{-1}$, $24.05(17) \times 10^{-6} \text{ K}^{-1}$, and $24.10(18) \times 10^{-6} \text{ K}^{-1}$ along the a , b , and c axes, respectively, at between 814 and 875 K.

Key words: structure determination; thermal expansion; solid oxide fuel cell

I. INTRODUCTION

Cobaltite perovskite oxides such as $(\text{La,Sr})\text{CoO}_{3-\delta}$ (LSC), $(\text{Sm,Sr})\text{CoO}_{3-\delta}$ (SSC) and $(\text{Ba,Sr})(\text{Co,Fe})\text{O}_{3-\delta}$ (BSCF) are mixed ionic/electronic conductors with high electrocatalytic activity to promote oxygen reduction required for their use as cathodes in solid-oxide fuel cells (Sun *et al.* 2009). Compared to LSC, SSC, with a smaller cation in the A site (Sm vs La), has been demonstrated to show much better oxygen surface exchange kinetics (Fukunaga *et al.* 2000). Therefore, SSC has been extensively investigated as a promising cathode material for intermediate-temperature solid oxide fuel cells (Dong *et al.* 2012; Ishihara *et al.* 1998; Tu *et al.* 1997; Xia *et al.* 2002; Yang *et al.* 2008).

The room-temperature structure of the SSC end-member, SmCoO_3 , has been studied previously in the context of solid-solution series with Ni (Pérez-Cacho *et al.* 2000), Fe (Kharko *et al.* 2014), and Sr (Tu *et al.* 1997), which, in all cases, was reported as the orthorhombic $Pbnm$ space-group (standard setting $Pnma$, no. 62 (Hahn 1995)). Tu *et al.* (1997) does report the rate of SmCoO_3 thermal expansion up to 1000 °C, however, this was measured on bulk, polycrystalline specimens, and reveals no information about any thermal expansion dependence on crystallographic parameters.

The aim of our research program is to investigate the atomic structure, thermal expansion behaviour, and electrochemical properties of various perovskites in order to correlate their structural parameters and behaviour as a solid-oxide fuel cell cathode. This work reports the temperature-dependent structure of SmCoO_3 from room temperature to 1245 K.

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II. EXPERIMENTAL

A. Sample Preparation

SmCoO_{3-δ} powder was synthesised by the combined citrate and ethylenediaminetetraacetic acid (EDTA) complexing method (Chen *et al.* 2016; Wang *et al.* 2009; Shao *et al.* 2012). The raw chemicals were Sm(NO₃)₃·6H₂O (99%, Sigma-Aldrich), Co(NO₃)₂·6H₂O (98.0% to 102.0%, Alfa-Aesar), citric acid (99.5%, Chem Supply), EDTA (99%, Acros Organics) and ammonia (28%, Ajax Finechem). The molar ratio of metal ions/citric acid/EDTA was 1:1.5:1. The resultant powder was calcined at 900 °C in air for 2 h.

B. In situ synchrotron X-ray powder diffraction

High-resolution X-ray powder diffraction patterns were collected using the Powder Diffraction beamline (Wallwork *et al.* 2007) at the Australian Synchrotron. A monochromatic X-ray beam with an energy of 15.5108 keV (determined from LaB₆ (NIST SRM 660b)) was used in order to keep away from the Sm L absorption edge to avoid spurious detector effects arising from specimen fluorescence. Data were collected over the angular range 3° to 83° 2θ using an array of Mythen position sensitive detector modules (Schmitt *et al.* 2003). To eliminate the gaps between the individual Mythen modules, the diffraction patterns were acquired in pairs with a goniometer rotation of 0.5° 2θ between each pattern, and merged using the program CONVAS2 (Rowles 2012). The SmCoO₃ powder was loaded in a 0.5 mm quartz capillary and mounted in Debye-Scherrer geometry. The capillary was continuously rotated about its long axis at ~1 Hz in order to provide even heating, improve particle statistics, and ensure accurate relative peak intensities.

The specimen was heated using a hot-air blower at a constant rate of 8 Kmin⁻¹ from room temperature up to 1245 K before cooling as rapidly as possible. The temperature was controlled by a thermocouple placed between the nozzle of the hot-air blower and the capillary. The specimen temperature was calibrated (Stinton and Evans 2007) using the known thermal expansion coefficients of corundum (Taylor 1984) applied to NIST SRM 676a. *In situ* diffraction patterns were collected for 45 s in each goniometer position, with approximately 13 s between each diffraction pattern for goniometer movement, for the duration of the experiment.

III. RESULTS AND DISCUSSION

Select diffraction patterns over the entire temperature range were indexed by the SVDIndex algorithm (Coelho 2003) in TOPAS (Bruker AXS 2014) and were all found to be consistent with the orthorhombic space-group *Pnma*, as has been found in previous room-temperature studies (Kharko *et al.* 2014; Pérez-Cacho *et al.* 2000; Tu *et al.* 1997). There were several unidentified minor impurity peaks present, but they were able to be discounted, as their thermal expansion behaviour was markedly different to that of the main perovskite phase.

All diffraction data were analysed by the Rietveld method (Rietveld 1969) as implemented in TOPAS. Refined parameters included background coefficients, specimen displacement (Scarlett *et al.* 2011), lattice parameters, profile coefficients, atomic position coordinates, and isotropic atomic displacement parameters. The zero offset was constrained to be the same over all patterns. The effect of specimen absorption and capillary geometry on peak intensities and profiles was modelled using a capillary aberration function based on the work of Sabine *et al.* (1998). The temperature calibration data were parametrically refined (Stinton and Evans 2007) to give the actual specimen temperature, which was then used unchanged. The isotropic displacement

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parameters of all atoms were found to vary quadratically with temperature, and were so constrained to this in the refinement, with only the coefficients of the quadratic being refined. Refinement of anisotropic displacement parameters was attempted, but was not found to be supported by the data.

The atomic positions were refined as distortion modes of a parent *Pm-3m* phase as given by the ISODISTORT suite (Campbell *et al.* 2006). The *Pnma* supercell is related to its parent by the transformation matrix $[[1\ 0\ 1],[0\ 2\ 0],[-1\ 0\ 1]]$, with its origin at (0,0,0). This structural transformation replaces the seven independent atomic position parameters of the *Pnma* space-group with seven distortion modes corresponding to two A-site cation displacements (R^+_5 (A) and X^+_5 (A)), two octahedral tilt/rotations about the *b* and *a* axes (M^+_3 (O) and R^+_4 (O)), and three octahedral distortions (M^+_2 (O), R^+_5 (O), and X^+_5 (O)), where X^+_5 (O) corresponds to a shear along the *a* axis.

The diffraction pattern and resultant Rietveld model for the data at 295 K are shown in Figure 1, with the refined structure shown in Figure 2. A summary of the structural parameters is given in Table I, showing that this material is isostructural with $GdFeO_3$ (Geller 1956). The supplemental information contains tables all of the structural data and the values in figures 3 – 7. To account for the contribution of the impurity phase, it was modelled as a set of peaks constrained by cubic *P-43n* symmetry, with changes in peak positions, intensity, and width with changes in temperature accommodated by refining a cell parameter, scale factor, and crystallite size parameter. The relative peak intensities of the impurity phase were fixed from refinement of the room-temperature model.

The orthorhombic symmetry of this perovskite can be explained as a distortion from the parent cubic perovskite phase ($a_p \approx 3.76$ Å) with tilts, rotations, and shears in the CoO_6 octahedra and translations of the Sm atom (Glazer 1975). The orthorhombic lattice parameters are given by $a \approx c \approx (\sqrt{2})a_p$ and $b \approx 2a_p$. No evidence was found for site occupancies of less than 100%, with all changes in intensity and peak position able to be described by changes in atom positions, unit cell parameters, and isotropic displacement parameters. There was no evidence of preferred orientation.

The temperature dependence of the distortion modes, as it influenced the Sm position and CoO_6 octahedral tilt, rotation, and shear are given in Figures 3 to 5. The data were denoised by numerical differentiation and antidifferentiation (Chartrand 2011), with $\alpha = 0.01$ for the translations and 0.05 for the octahedral distortions. Both the A-site translational distortions, R^+_5 (A) and X^+_5 (A), were found to be significant. Only the octahedral M^+_3 (O), R^+_4 (O), and X^+_5 (O) distortions were found to be significant, with the negligible M^+_2 (O) and R^+_5 (O) distortions fixed at zero. The R^+_4 (O) distortion is a tilting of the CoO_6 octahedra about the *a* direction, and the M^+_3 (O) distortion is a rotation of the octahedra about the *b* direction. The X^+_5 (O) distortion is a shearing of the apical oxygen of the CoO_6 octahedra in the *a* direction. The distortion magnitudes were converted to fractional coordinates and tilt/rotation/shear angles by the following formulae:

$$\begin{aligned} \text{Sm } x &= \frac{1}{2} + 0.09399X_5^+ \\ \text{Sm } z &= 0.09399R_5^+ \end{aligned}$$

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$$\text{Oct. rot.} = \arctan \left[\frac{0.06646R_4^+ c}{\frac{1}{4}b} \right]$$

$$\text{Oct. tilt} = \arctan \left[\frac{a \left(-\frac{1}{4} - 0.04699M_3^+ \right)}{c \left(\frac{1}{4} - 0.04699M_3^+ \right)} \right]$$

$$\text{Oct. shear} = \arctan \left[\frac{0.09399X_5^+ a}{\frac{1}{4}b} \right]$$

where the decimal values were given by the output of the ISODISTORT suite (Campbell *et al.* 2006).

The A-site translational distortions are anticorrelated, with the Sm atom moving diagonally in the xz plane with changes in temperature. The octahedral tilt and rotation also tend to occur in opposite directions; as the tilt increases, the rotation decreases. The octahedral shear appears to follow the same behaviour as the octahedral tilt, but leading those changes by about 140 K.

The temperature dependence of the unit cell parameters is shown in Figure 6. Both the instantaneous and average linear thermal expansion coefficients (TECs) are shown in Figure 7, clearly showing both their non-linearity and anisotropy. The instantaneous and average TECs were calculated as

$$\text{TEC}_{\text{inst.}} = \frac{1}{l} \frac{dl}{dT}$$

$$\text{TEC}_{\text{ave}} = \frac{1}{l_0} \frac{\Delta l}{\Delta T}$$

where l and l_0 are the current and initial cell parameters, respectively, and Δ represents the difference between the current value of the cell parameter or temperature and its initial value. The derivative was calculated numerically (Chartrand 2011). The bulk TECs calculated from the data of Tu *et al.* (1997) are also given for comparison. The maximum instantaneous and average TECs are given in Table II.

Overall, the unit cell expands much more in the a direction than in the b and c directions, where the expansion is essentially equal. The peak average TEC in the a direction occurs at approximately 800 K, which is well within the operating range of intermediate-temperature solid-oxide fuel cells (Brett *et al.* 2008), and is much greater than any of the values given by (Sun *et al.* 2009). Above this temperature, the thermal expansion is still non-linear, but to a greatly reduced degree. Comparison of the average TECs to the bulk TECs of Tu *et al.* (1997) show that a simple average of the TECs of the three crystallographic directions can explain the bulk measurements.

The large anisotropy and non-linearity in the TECs below 900 K has implications for the structural integrity of polycrystalline monoliths and for joints between different solid-oxide fuel cell components, as repeated temperature cycling may induce cracking and delamination. The point of greatest orthorhombic distortion occurs at ~ 1000 K, where the instantaneous TECs cross over.

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The maximum of the instantaneous TEC for all three axes occurs at ~640 K, showing that the gross relative changes in the average TEC for all three axes are the same.

IV. CONCLUSIONS

The structure and thermal expansion of the perovskite SmCoO_3 has been determined over the temperature range 295 to 1245 K. The structure was found to be orthorhombic ($Pnma$) and isostructural with GdFeO_3 over the entire temperature range. The thermal expansion is both non-linear and anisotropic with a maximum average linear thermal expansion coefficient of $34.0(3) \times 10^{-6} \text{ K}^{-1}$, $24.05(17) \times 10^{-6} \text{ K}^{-1}$, and $24.10(18) \times 10^{-6} \text{ K}^{-1}$ along the a , b , and c axes, respectively, between 814 and 875 K. Structural information is available in the supplemental information and select temperatures have been uploaded to the Crystallography Online Database.

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Figure captions

FIG. 1. Diffraction data and Rietveld model of SmCoO_3 at 295 K. Data was collected over the range 3 to $83^\circ 2\theta$.

FIG. 2. The structure of SmCoO_3 at 295 K. The images clearly show the tilt and rotation of the CoO_6 corner-sharing octahedra, as well as the offset of the Sm atoms from the face of the unit cell. Distortion of the octahedra is minimal.

FIG. 3. Sm fractional x and z coordinates as a function of temperature. The R_5^+ and X_5^+ distortions correspond to translations of the Sm atom in the z and x directions, respectively. The solid line is the denoised data. Error bars are given for every third data point and represent one estimated standard deviation.

FIG. 4. CoO_6 octahedral tilt and rotation distortion as a function of temperature. The solid line is the denoised data. Error bars are given for every third data point and represent one estimated standard deviation.

FIG. 5. CoO_6 octahedral shear distortion as a function of temperature. The solid line is the denoised data. Error bars are given for every third data point and represent one estimated standard deviation.

FIG. 6. Unit cell parameters as a function of temperature. The non-linear expansion behaviour of all three axes is clear. The error bars are smaller than the data points. $b' = b/\sqrt{2}$.

Fig. 7. Instantaneous (I) and average (A) linear thermal expansion coefficients (TECs) for the three cell parameters showing the expansion anisotropy. The open circles are bulk TECs calculated from the results of Tu *et al.* (1997). The point of maximum orthorhombic distortion occurs at the high temperature crossover of the instantaneous coefficients at ~ 1000 K.

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Tables

Table I. Crystal data for SmCoO₃ at select temperatures. Space group *Pnma*, Z = 4. Molar mass = 257.29 g mol⁻¹. By space group symmetry, Sm y & O2 y = ¼, and Co x; y; z = 0; 0; 0. The structure data for the remaining temperatures is available in the supplemental information

	295 K	830 K	1245 K
a (Å)	5.362267(12)	5.459411(10)	5.505157(13)
b (Å)	7.510380(14)	7.606208(12)	7.67164(2)
c (Å)	5.292981(11)	5.360822(9)	5.405593(17)
Volume (Å ³)	213.1624(8)	222.6103(7)	228.2975(11)
Density (g cm ⁻³)	8.01722(3)	7.67696(2)	7.48572(4)
Sm x	0.54748(5)	0.54723(7)	0.54586(6)
Sm z	-0.00970(5)	-0.00937(7)	-0.00881(10)
O1 x	0.2919(5)	0.2938(5)	0.2932(6)
O1 y	0.0414(3)	0.0406(3)	0.0410(4)
O1 z	0.7919(5)	0.7938(5)	0.7932(6)
O2 x	-0.0162(1)	-0.0173(1)	-0.0135(8)
O2 z	0.0828(6)	0.0812(5)	0.0820(8)
Sm B (Å ²)	0.7119(5)	1.7016(8)	2.4282(15)
Co B (Å ²)	0.5333(13)	1.0966(18)	1.542(3)
O1 B (Å ²)	0.526(5)	1.822(5)	2.838(7)
O2 B (Å ²)	0.835(8)	1.937(9)	2.578(13)

Table II. Maximum instantaneous and average thermal expansion coefficients and their respective temperatures and crystallographic direction. The uncertainties incorporate a coverage factor of 2 and the uncertainties were estimated from the magnitudes of the average uncertainties.

Axis	Instantaneous (x10 ⁻⁶ K ⁻¹)	Temperature (K)	Average (x10 ⁻⁶ K ⁻¹)	Temperature (K)
a	54.5(6)	640	34.0(3)	814
b	33.5(4)	656	24.05(17)	875
c	33.1(4)	640	24.10(18)	845

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Supplementary information

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Table SI. Lattice parameters, volume, and density for SmCoO₃ at all temperatures. Space group *Pnma*, Z = 4. Molar mass = 257.29 g mol⁻¹.

Temp. (K)	a (Å)	b (Å)	c (Å)	vol. (Å ³)	dens. (g/cm ³)
295	5.362267(12)	7.510380(14)	5.292981(11)	213.1624(8)	8.01722(3)
315	5.362750(13)	7.511722(13)	5.293965(12)	213.2594(8)	8.01358(3)
332	5.363407(13)	7.513198(14)	5.295079(10)	213.3723(8)	8.00934(3)
350	5.364257(13)	7.514790(13)	5.296299(12)	213.5005(8)	8.00453(3)
368	5.365335(14)	7.516596(13)	5.297619(10)	213.6480(8)	7.99900(3)
386	5.366736(14)	7.518513(14)	5.299061(11)	213.8165(8)	7.99270(3)
403	5.368338(14)	7.520568(15)	5.300603(11)	214.0010(8)	7.98581(3)
421	5.370148(15)	7.522760(15)	5.302248(11)	214.2020(8)	7.97831(3)
439	5.372432(15)	7.525280(15)	5.304110(11)	214.4401(9)	7.96945(3)
455	5.374787(14)	7.527772(15)	5.305972(10)	214.6805(8)	7.96053(3)
473	5.377486(16)	7.530458(13)	5.307942(11)	214.9448(9)	7.95074(3)
490	5.380379(15)	7.533347(13)	5.310039(10)	215.2279(8)	7.94029(3)
507	5.383488(15)	7.536317(14)	5.312201(12)	215.5249(9)	7.92934(3)
524	5.386789(15)	7.539428(14)	5.314421(11)	215.8362(8)	7.91791(3)
541	5.390087(18)	7.542522(13)	5.316657(10)	216.1479(9)	7.90649(3)
558	5.393918(15)	7.545908(13)	5.319116(11)	216.4987(8)	7.89368(3)
575	5.397829(16)	7.549416(14)	5.321627(11)	216.8587(9)	7.88057(3)
591	5.401923(16)	7.553011(14)	5.324188(11)	217.2310(9)	7.86707(3)
608	5.406215(15)	7.556727(14)	5.326876(11)	217.6204(8)	7.85299(3)
624	5.410817(13)	7.560650(13)	5.329638(11)	218.0317(8)	7.83818(3)
640	5.415360(13)	7.564535(13)	5.332335(11)	218.4374(8)	7.82362(3)
656	5.420069(13)	7.568523(13)	5.335119(12)	218.8568(8)	7.80863(3)
673	5.424780(13)	7.572557(13)	5.337906(11)	219.2783(8)	7.79362(3)
689	5.429538(12)	7.576698(12)	5.340777(11)	219.7087(8)	7.77835(3)
705	5.433665(11)	7.580402(10)	5.343311(11)	220.0876(7)	7.76496(2)
721	5.437758(13)	7.584137(13)	5.345880(10)	220.4679(8)	7.75156(3)
737	5.441235(12)	7.587412(11)	5.348113(10)	220.7963(7)	7.74003(2)
752	5.444670(11)	7.590678(13)	5.350340(10)	221.1228(7)	7.72861(2)
768	5.447469(12)	7.593431(13)	5.352210(10)	221.3941(7)	7.71914(3)
783	5.450935(13)	7.596998(13)	5.354632(10)	221.7393(8)	7.70712(3)
799	5.453631(11)	7.599788(14)	5.356509(11)	222.0082(8)	7.69778(3)
814	5.456938(10)	7.603417(12)	5.358958(10)	222.3505(7)	7.68593(2)
830	5.459411(10)	7.606208(12)	5.360822(9)	222.6103(7)	7.67696(2)
845	5.462339(9)	7.609539(12)	5.363080(9)	222.9211(6)	7.66626(2)
860	5.464453(9)	7.611987(13)	5.364712(9)	223.1470(7)	7.65850(2)
875	5.467000(9)	7.615058(13)	5.366799(10)	223.4280(7)	7.64887(2)
889	5.469117(9)	7.617661(15)	5.368576(10)	223.6650(7)	7.64076(2)

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904	5.471187(10)	7.620258(13)	5.370311(9)	223.8982(7)	7.63280(2)
919	5.473089(10)	7.622650(14)	5.371919(10)	224.1135(7)	7.62547(2)
934	5.474805(10)	7.624891(14)	5.373453(11)	224.3137(8)	7.61866(3)
948	5.477068(10)	7.627873(14)	5.375452(10)	224.5776(7)	7.60971(2)
963	5.478677(9)	7.630062(14)	5.376942(11)	224.7704(7)	7.60318(2)
977	5.480447(9)	7.632521(13)	5.378571(10)	224.9836(7)	7.59598(2)
991	5.482013(10)	7.634692(15)	5.380069(11)	225.1746(8)	7.58954(3)
1005	5.483778(9)	7.637130(15)	5.381728(11)	225.3885(8)	7.58233(3)
1019	5.485170(9)	7.639168(15)	5.383113(11)	225.5640(7)	7.57644(3)
1034	5.486466(10)	7.641077(17)	5.384421(12)	225.7284(8)	7.57092(3)
1048	5.487968(9)	7.643280(15)	5.385927(10)	225.9185(7)	7.56455(2)
1061	5.489331(9)	7.645302(17)	5.387313(10)	226.0926(8)	7.55872(3)
1076	5.490659(10)	7.647310(18)	5.388670(12)	226.2636(8)	7.55301(3)
1089	5.491902(11)	7.649258(19)	5.390011(13)	226.4288(9)	7.54750(3)
1103	5.493166(11)	7.651246(18)	5.391391(12)	226.5978(9)	7.54187(3)
1116	5.494448(9)	7.653327(18)	5.392807(12)	226.7718(8)	7.53608(3)
1130	5.495533(11)	7.655029(18)	5.394009(12)	226.9177(9)	7.53124(3)
1142	5.496933(11)	7.657297(19)	5.395592(12)	227.1093(9)	7.52488(3)
1156	5.497982(11)	7.659079(20)	5.396800(12)	227.2564(9)	7.52001(3)
1169	5.499181(12)	7.661091(20)	5.398208(14)	227.4250(10)	7.51444(3)
1181	5.500281(11)	7.662970(20)	5.399508(15)	227.5811(10)	7.50928(3)
1195	5.501171(13)	7.664560(21)	5.400625(14)	227.7123(10)	7.50496(3)
1207	5.502118(12)	7.666162(24)	5.401748(15)	227.8464(11)	7.50054(4)
1220	5.503401(14)	7.668478(22)	5.403385(15)	228.0375(11)	7.49425(4)
1233	5.504310(12)	7.670106(23)	5.404561(14)	228.1732(10)	7.48980(3)
1245	5.505157(13)	7.671638(24)	5.405593(17)	228.2975(11)	7.48572(4)

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Table SII. Atom positions for SmCoO₃ at all temperatures. Space group *Pnma*, Z = 4. Molar mass = 257.29 g mol⁻¹. By space group symmetry, Sm *y* & O2 *y* = ¼, and Co *x*; *y*; *z* = 0; 0; 0.

Temp. (K)	Sm_x	Sm_z	O1_x	O1_y	O1_z	O2_x	O2_z
295	0.54748(5)	-0.00970(5)	0.2919(5)	0.0414(3)	0.7919(5)	-0.0162(10)	0.0828(6)
315	0.54736(6)	-0.00957(6)	0.2921(5)	0.0412(3)	0.7921(5)	-0.0165(9)	0.0825(5)
332	0.54722(6)	-0.00958(6)	0.2919(5)	0.0414(3)	0.7919(5)	-0.0172(9)	0.0828(5)
350	0.54709(6)	-0.00950(6)	0.2919(5)	0.0416(3)	0.7919(5)	-0.0178(10)	0.0831(5)
368	0.54697(6)	-0.00944(5)	0.2919(5)	0.0413(3)	0.7919(5)	-0.0169(10)	0.0826(6)
386	0.54689(6)	-0.00937(5)	0.2918(5)	0.0415(3)	0.7918(5)	-0.0168(10)	0.0829(5)
403	0.54673(6)	-0.00932(6)	0.2918(5)	0.0413(3)	0.7918(5)	-0.0170(10)	0.0826(5)
421	0.54671(6)	-0.00917(5)	0.2919(5)	0.0415(3)	0.7919(5)	-0.0166(11)	0.0830(5)
439	0.54662(7)	-0.00911(6)	0.2922(5)	0.0414(3)	0.7922(5)	-0.0169(11)	0.0828(6)
455	0.54656(6)	-0.00915(6)	0.2921(6)	0.0414(3)	0.7921(6)	-0.0168(11)	0.0828(6)
473	0.54651(6)	-0.00900(6)	0.2922(5)	0.0411(3)	0.7922(5)	-0.0178(10)	0.0822(5)
490	0.54652(6)	-0.00904(6)	0.2922(5)	0.0413(3)	0.7922(5)	-0.0178(11)	0.0826(6)
507	0.54650(7)	-0.00891(6)	0.2921(5)	0.0415(3)	0.7921(5)	-0.0183(11)	0.0830(6)
524	0.54655(6)	-0.00890(6)	0.2920(5)	0.0414(3)	0.7920(5)	-0.0190(10)	0.0828(5)
541	0.54654(7)	-0.00897(7)	0.2917(6)	0.0412(3)	0.7917(6)	-0.0196(12)	0.0824(5)
558	0.54653(7)	-0.00894(7)	0.2916(5)	0.0415(3)	0.7916(5)	-0.0196(11)	0.0829(6)
575	0.54650(7)	-0.00901(7)	0.2921(5)	0.0413(3)	0.7921(5)	-0.0188(11)	0.0826(6)
591	0.54644(7)	-0.00909(7)	0.2922(6)	0.0411(3)	0.7922(6)	-0.0165(13)	0.0823(6)
608	0.54666(7)	-0.00914(6)	0.2920(6)	0.0415(3)	0.7920(6)	-0.0184(12)	0.0831(6)
624	0.54670(8)	-0.00915(7)	0.2922(5)	0.0413(3)	0.7922(5)	-0.0179(12)	0.0826(6)
640	0.54668(8)	-0.00912(6)	0.2926(5)	0.0415(3)	0.7926(5)	-0.0163(11)	0.0830(6)
656	0.54684(7)	-0.00912(7)	0.2931(5)	0.0419(3)	0.7931(5)	-0.0164(11)	0.0837(6)
673	0.54696(7)	-0.00910(7)	0.2931(6)	0.0418(3)	0.7931(6)	-0.0149(13)	0.0837(6)
689	0.54707(7)	-0.00921(7)	0.2932(5)	0.0416(3)	0.7932(5)	-0.0130(12)	0.0833(6)
705	0.54712(7)	-0.00913(7)	0.2938(5)	0.0414(3)	0.7938(5)	-0.0136(12)	0.0828(7)
721	0.54725(7)	-0.00917(7)	0.2934(6)	0.0416(3)	0.7934(6)	-0.0149(14)	0.0832(6)
737	0.54712(7)	-0.00920(6)	0.2936(5)	0.0412(3)	0.7936(5)	-0.0163(12)	0.0824(6)
752	0.54724(8)	-0.00934(7)	0.2945(5)	0.0412(3)	0.7945(5)	-0.0158(12)	0.0823(5)
768	0.54733(7)	-0.00922(7)	0.2935(5)	0.0415(3)	0.7935(5)	-0.0155(13)	0.0830(6)
783	0.54720(7)	-0.00937(6)	0.2941(5)	0.0411(3)	0.7941(5)	-0.0162(11)	0.0821(5)
799	0.54730(7)	-0.00929(7)	0.2938(5)	0.0408(3)	0.7938(5)	-0.0169(11)	0.0817(5)
814	0.54733(7)	-0.00943(7)	0.2940(4)	0.0407(2)	0.7940(4)	-0.0166(11)	0.0814(5)
830	0.54723(7)	-0.00937(7)	0.2938(5)	0.0406(3)	0.7938(5)	-0.0173(10)	0.0812(5)
845	0.54737(7)	-0.00948(6)	0.2941(4)	0.0407(3)	0.7941(4)	-0.0167(10)	0.0813(5)
860	0.54723(6)	-0.00929(6)	0.2939(5)	0.0407(3)	0.7939(5)	-0.0164(10)	0.0813(5)
875	0.54734(7)	-0.00937(6)	0.2940(5)	0.0407(2)	0.7940(5)	-0.0156(10)	0.0814(5)
889	0.54727(6)	-0.00957(6)	0.2940(4)	0.0406(3)	0.7940(4)	-0.0166(9)	0.0812(5)

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904	0.54720(6)	-0.00931(7)	0.2936(5)	0.0410(2)	0.7936(5)	-0.0161(10)	0.0819(4)
919	0.54727(6)	-0.00939(7)	0.2939(4)	0.0408(3)	0.7939(4)	-0.0154(9)	0.0817(5)
934	0.54728(6)	-0.00936(7)	0.2934(4)	0.0408(3)	0.7934(4)	-0.0170(10)	0.0816(6)
948	0.54713(6)	-0.00937(7)	0.2938(4)	0.0407(2)	0.7938(4)	-0.0162(9)	0.0815(5)
963	0.54715(6)	-0.00932(7)	0.2936(5)	0.0410(3)	0.7936(5)	-0.0162(9)	0.0820(5)
977	0.54702(6)	-0.00920(7)	0.2933(4)	0.0411(3)	0.7933(4)	-0.0162(9)	0.0822(5)
991	0.54702(6)	-0.00913(7)	0.2937(4)	0.0410(2)	0.7937(4)	-0.0161(9)	0.0819(5)
1005	0.54698(5)	-0.00908(7)	0.2927(5)	0.0410(3)	0.7927(5)	-0.0154(8)	0.0821(5)
1019	0.54698(6)	-0.00922(7)	0.2931(5)	0.0410(3)	0.7931(5)	-0.0147(8)	0.0819(5)
1034	0.54692(6)	-0.00907(7)	0.2930(5)	0.0412(3)	0.7930(5)	-0.0154(8)	0.0824(5)
1048	0.54687(6)	-0.00913(7)	0.2933(5)	0.0412(3)	0.7933(5)	-0.0157(7)	0.0824(5)
1061	0.54680(6)	-0.00910(8)	0.2927(4)	0.0412(3)	0.7927(4)	-0.0153(8)	0.0824(6)
1076	0.54681(5)	-0.00908(7)	0.2930(5)	0.0412(3)	0.7930(5)	-0.0149(7)	0.0823(6)
1089	0.54675(6)	-0.00909(8)	0.2930(4)	0.0411(3)	0.7930(4)	-0.0141(8)	0.0821(6)
1103	0.54666(5)	-0.00914(8)	0.2930(5)	0.0409(3)	0.7930(5)	-0.0143(7)	0.0819(6)
1116	0.54661(5)	-0.00893(8)	0.2929(5)	0.0412(3)	0.7929(5)	-0.0133(8)	0.0825(6)
1130	0.54657(6)	-0.00913(7)	0.2936(5)	0.0410(3)	0.7936(5)	-0.0131(7)	0.0821(6)
1142	0.54642(5)	-0.00904(8)	0.2930(5)	0.0409(3)	0.7930(5)	-0.0135(8)	0.0818(6)
1156	0.54640(6)	-0.00905(8)	0.2927(6)	0.0410(3)	0.7927(6)	-0.0127(8)	0.0819(6)
1169	0.54635(5)	-0.00900(9)	0.2930(5)	0.0412(3)	0.7930(5)	-0.0127(7)	0.0823(6)
1181	0.54631(5)	-0.00894(9)	0.2929(5)	0.0411(3)	0.7929(5)	-0.0122(7)	0.0821(6)
1195	0.54623(5)	-0.00881(8)	0.2928(5)	0.0410(3)	0.7928(5)	-0.0137(7)	0.0819(6)
1207	0.54611(5)	-0.00889(9)	0.2927(6)	0.0411(4)	0.7927(6)	-0.0124(8)	0.0822(7)
1220	0.54598(6)	-0.00908(9)	0.2932(6)	0.0407(3)	0.7932(6)	-0.0133(7)	0.0814(7)
1233	0.54607(6)	-0.00916(9)	0.2926(6)	0.0405(4)	0.7926(6)	-0.0129(7)	0.0810(7)
1245	0.54586(6)	-0.00881(10)	0.2932(6)	0.0410(4)	0.7932(6)	-0.0135(8)	0.0820(8)

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Table SIII. Isotropic thermal parameters for SmCoO₃ at all temperatures.

Temp. (K)	Sm _{beq} (Å ²)	Co _{beq} (Å ²)	O1 _{beq} (Å ²)	O2 _{beq} (Å ²)
295	0.7119(5)	0.5333(13)	0.526(5)	0.835(8)
315	0.7488(5)	0.5536(13)	0.573(5)	0.880(8)
332	0.7823(5)	0.5719(13)	0.615(5)	0.921(8)
350	0.8161(5)	0.5905(13)	0.658(5)	0.962(8)
368	0.8497(5)	0.6091(13)	0.701(5)	1.003(8)
386	0.8842(5)	0.6281(13)	0.745(5)	1.044(8)
403	0.9160(5)	0.6458(13)	0.786(5)	1.082(8)
421	0.9500(5)	0.6647(13)	0.829(5)	1.122(8)
439	0.9833(5)	0.6833(13)	0.872(5)	1.161(8)
455	1.0151(5)	0.7011(13)	0.913(5)	1.198(8)
473	1.0470(6)	0.7190(13)	0.954(5)	1.235(8)
490	1.0798(6)	0.7374(13)	0.997(5)	1.273(8)
507	1.1115(6)	0.7553(14)	1.038(5)	1.309(8)
524	1.1434(6)	0.7733(14)	1.079(5)	1.345(8)
541	1.1743(6)	0.7908(14)	1.120(5)	1.380(8)
558	1.2063(6)	0.8090(14)	1.161(5)	1.416(8)
575	1.2368(6)	0.8263(14)	1.201(5)	1.450(8)
591	1.2679(6)	0.8441(14)	1.242(5)	1.484(8)
608	1.2979(6)	0.8613(14)	1.282(5)	1.517(8)
624	1.3273(6)	0.8781(15)	1.320(5)	1.549(8)
640	1.3581(6)	0.8959(15)	1.361(5)	1.582(8)
656	1.3873(6)	0.9127(15)	1.400(5)	1.614(8)
673	1.4175(7)	0.9302(15)	1.440(5)	1.646(8)
689	1.4462(7)	0.9468(15)	1.478(5)	1.676(8)
705	1.4763(7)	0.9643(16)	1.518(5)	1.708(8)
721	1.5042(7)	0.9805(16)	1.555(5)	1.737(8)
737	1.5337(7)	0.9978(16)	1.595(5)	1.768(8)
752	1.5615(7)	1.0141(16)	1.632(5)	1.796(8)
768	1.5902(7)	1.0309(16)	1.671(5)	1.825(8)
783	1.6180(7)	1.0472(17)	1.708(5)	1.854(9)
799	1.6463(8)	1.0639(17)	1.747(5)	1.882(9)
814	1.6734(8)	1.0800(17)	1.783(5)	1.909(9)
830	1.7016(8)	1.0966(18)	1.822(5)	1.937(9)
845	1.7280(8)	1.1123(18)	1.857(5)	1.963(9)
860	1.7558(8)	1.1288(18)	1.895(6)	1.990(9)
875	1.7819(9)	1.1444(18)	1.931(6)	2.015(9)
889	1.8080(9)	1.1601(19)	1.967(6)	2.040(9)
904	1.8348(9)	1.1761(19)	2.003(6)	2.066(9)

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919	1.8605(9)	1.1916(19)	2.039(6)	2.090(9)
934	1.8869(9)	1.207(2)	2.075(6)	2.115(9)
948	1.9122(10)	1.223(2)	2.110(6)	2.139(9)
963	1.9383(10)	1.238(2)	2.146(6)	2.163(10)
977	1.9632(10)	1.254(2)	2.181(6)	2.186(10)
991	1.9877(10)	1.268(2)	2.215(6)	2.208(10)
1005	2.0132(10)	1.284(2)	2.250(6)	2.231(10)
1019	2.0373(11)	1.299(2)	2.284(6)	2.253(10)
1034	2.0624(11)	1.314(2)	2.319(6)	2.275(10)
1048	2.0874(11)	1.329(2)	2.354(6)	2.297(10)
1061	2.1108(11)	1.344(2)	2.387(6)	2.317(10)
1076	2.1356(12)	1.359(2)	2.421(6)	2.339(11)
1089	2.1584(12)	1.373(2)	2.453(7)	2.358(11)
1103	2.1828(12)	1.388(2)	2.488(7)	2.379(11)
1116	2.2057(12)	1.402(3)	2.520(7)	2.399(11)
1130	2.2293(13)	1.417(3)	2.554(7)	2.418(11)
1142	2.2516(13)	1.431(3)	2.585(7)	2.437(11)
1156	2.2750(13)	1.446(3)	2.619(7)	2.456(11)
1169	2.2970(13)	1.459(3)	2.650(7)	2.474(12)
1181	2.3187(14)	1.473(3)	2.681(7)	2.492(12)
1195	2.3417(14)	1.487(3)	2.714(7)	2.510(12)
1207	2.3628(14)	1.501(3)	2.744(7)	2.527(12)
1220	2.3853(15)	1.515(3)	2.776(7)	2.545(12)
1233	2.4065(15)	1.528(3)	2.807(7)	2.561(12)
1245	2.4282(15)	1.542(3)	2.838(7)	2.578(13)

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Table SIV. Octahedral tilt, rotation, and shear for CoO₆ at all temperatures.

Temp. (K)	Tilt (°)	Rotation (°)	Shear (°)
295	13.13(8)	9.15(7)	2.65(17)
315	13.09(8)	9.22(7)	2.70(15)
332	13.13(8)	9.16(7)	2.81(14)
350	13.19(8)	9.16(8)	2.91(16)
368	13.11(8)	9.16(8)	2.76(16)
386	13.16(8)	9.16(8)	2.74(16)
403	13.12(8)	9.15(7)	2.77(17)
421	13.18(8)	9.18(7)	2.72(19)
439	13.13(9)	9.24(8)	2.77(18)
455	13.14(9)	9.21(8)	2.74(18)
473	13.04(8)	9.22(8)	2.91(17)
490	13.11(9)	9.22(8)	2.91(17)
507	13.17(9)	9.19(8)	2.99(18)
524	13.13(8)	9.18(7)	3.12(17)
541	13.08(8)	9.10(8)	3.2(2)
558	13.16(9)	9.07(7)	3.21(18)
575	13.11(9)	9.17(8)	3.09(18)
591	13.06(9)	9.18(9)	2.7(2)
608	13.18(9)	9.13(8)	3.0(2)
624	13.11(10)	9.17(8)	2.9(2)
640	13.18(9)	9.25(7)	2.68(19)
656	13.28(10)	9.36(8)	2.69(18)
673	13.27(9)	9.35(8)	2.4(2)
689	13.21(9)	9.36(7)	2.14(19)
705	13.14(10)	9.48(7)	2.2(2)
721	13.20(10)	9.39(8)	2.4(2)
737	13.09(8)	9.43(7)	2.68(19)
752	13.06(8)	9.61(7)	2.6(2)
768	13.16(9)	9.39(7)	2.5(2)
783	13.04(8)	9.52(7)	2.67(18)
799	12.96(8)	9.46(7)	2.78(18)
814	12.93(8)	9.50(6)	2.74(19)
830	12.90(8)	9.44(7)	2.84(17)
845	12.91(8)	9.51(6)	2.74(16)
860	12.91(8)	9.47(7)	2.70(17)
875	12.92(7)	9.48(7)	2.56(16)
889	12.90(8)	9.47(6)	2.72(15)
904	13.00(7)	9.38(7)	2.65(17)

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919	12.97(8)	9.45(6)	2.54(16)
934	12.95(9)	9.34(6)	2.80(16)
948	12.94(8)	9.42(6)	2.66(14)
963	13.02(8)	9.40(7)	2.66(15)
977	13.04(8)	9.33(6)	2.67(15)
991	13.00(7)	9.41(6)	2.65(14)
1005	13.03(8)	9.19(7)	2.54(14)
1019	13.00(8)	9.26(7)	2.41(14)
1034	13.08(8)	9.26(7)	2.53(13)
1048	13.08(8)	9.31(7)	2.58(11)
1061	13.07(9)	9.19(6)	2.51(13)
1076	13.07(9)	9.25(7)	2.46(12)
1089	13.03(9)	9.24(6)	2.32(13)
1103	13.00(9)	9.24(7)	2.36(12)
1116	13.09(10)	9.24(8)	2.19(14)
1130	13.02(9)	9.39(7)	2.16(12)
1142	12.98(10)	9.26(7)	2.23(13)
1156	13.01(10)	9.19(8)	2.09(13)
1169	13.06(10)	9.26(8)	2.09(12)
1181	13.03(10)	9.23(7)	2.00(12)
1195	13.01(9)	9.22(8)	2.25(12)
1207	13.04(11)	9.20(9)	2.04(13)
1220	12.92(10)	9.32(8)	2.19(12)
1233	12.86(11)	9.18(8)	2.13(11)
1245	13.01(12)	9.31(8)	2.22(12)

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Table SV. Instantaneous and average linear thermal expansion coefficients for SmCoO₃ at all temperatures.

Temp. (K)	ILTEC_a (x10 ⁻⁶ K ⁻¹)	ILTEC_b (x10 ⁻⁶ K ⁻¹)	ILTEC_c (x10 ⁻⁶ K ⁻¹)	ALTEC_a (x10 ⁻⁶ K ⁻¹)	ALTEC_b (x10 ⁻⁶ K ⁻¹)	ALTEC_c (x10 ⁻⁶ K ⁻¹)
315	5.8(6)	9.3(10)	9.9(10)	4.6(5)	9.2(10)	9.6(10)
332	8.2(5)	11.3(6)	12.0(7)	5.8(3)	10.2(6)	10.7(6)
350	11.0(4)	13.3(5)	14.1(5)	6.8(3)	10.7(4)	11.4(4)
368	14.2(4)	15.2(4)	16.1(4)	7.9(2)	11.4(3)	12.1(3)
386	17.4(4)	16.9(4)	17.9(4)	9.2(2)	11.9(3)	12.7(3)
403	20.7(4)	18.4(3)	19.5(4)	10.5(2)	12.6(2)	13.4(3)
421	24.0(4)	19.8(3)	20.9(3)	11.70(19)	13.1(2)	13.9(2)
439	27.1(4)	21.1(3)	22.2(3)	13.22(19)	13.84(19)	14.7(2)
455	30.0(4)	22.3(3)	23.4(3)	14.57(18)	14.45(18)	15.31(19)
473	32.8(4)	23.5(3)	24.4(3)	16.00(18)	15.07(17)	15.93(18)
490	35.4(4)	24.6(3)	25.4(3)	17.33(18)	15.69(16)	16.53(17)
507	37.9(4)	25.7(2)	26.4(3)	18.67(18)	16.29(15)	17.13(16)
524	40.4(4)	26.8(2)	27.5(2)	19.96(17)	16.88(15)	17.68(15)
541	42.9(4)	27.9(2)	28.5(2)	21.12(17)	17.42(14)	18.20(15)
558	45.5(3)	29.1(2)	29.6(2)	22.44(17)	17.99(14)	18.78(14)
575	48.0(3)	30.2(2)	30.7(2)	23.73(17)	18.60(13)	19.37(14)
591	50.4(3)	31.3(2)	31.6(2)	24.96(17)	19.16(13)	19.90(13)
608	52.4(3)	32.2(2)	32.4(2)	26.22(17)	19.74(13)	20.49(13)
624	53.8(3)	33.0(2)	32.9(2)	27.56(17)	20.37(12)	21.08(13)
640	54.5(3)	33.40(19)	33.12(19)	28.67(17)	20.88(12)	21.53(12)
656	54.4(3)	33.48(19)	33.02(18)	29.84(17)	21.43(12)	22.04(12)
673	53.3(3)	33.13(18)	32.52(17)	30.86(16)	21.91(12)	22.47(12)
689	51.2(3)	32.30(16)	31.58(16)	31.88(16)	22.44(11)	22.95(12)
705	48.4(2)	31.11(15)	30.30(15)	32.47(16)	22.74(11)	23.19(11)
721	45.2(2)	29.77(14)	28.90(14)	33.10(16)	23.09(11)	23.50(11)
737	42.09(19)	28.50(13)	27.58(13)	33.35(15)	23.22(11)	23.59(11)
752	39.42(17)	27.52(12)	26.55(12)	33.63(15)	23.40(10)	23.71(10)
768	37.34(16)	26.91(11)	25.88(11)	33.60(14)	23.39(10)	23.67(10)
783	35.67(15)	26.54(11)	25.45(10)	33.87(14)	23.62(10)	23.86(10)
799	34.19(14)	26.23(10)	25.10(10)	33.81(13)	23.62(9)	23.82(9)
814	32.70(13)	25.82(10)	24.68(10)	34.02(13)	23.87(9)	24.02(9)
830	31.13(12)	25.23(9)	24.11(9)	33.88(13)	23.86(9)	23.97(9)
845	29.49(11)	24.49(9)	23.42(9)	33.96(12)	24.03(9)	24.10(9)
860	27.88(10)	23.71(8)	22.69(8)	33.73(12)	23.95(8)	23.99(9)
875	26.37(9)	22.94(8)	21.96(8)	33.70(12)	24.05(8)	24.06(8)
889	24.96(8)	22.18(7)	21.24(7)	33.53(11)	24.04(8)	24.03(8)
904	23.74(8)	21.54(7)	20.63(7)	33.33(11)	24.01(8)	23.98(8)

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919	22.75(7)	21.06(7)	20.18(6)	33.13(11)	23.96(8)	23.91(8)
934	21.97(7)	20.74(7)	19.87(6)	32.86(10)	23.87(7)	23.80(7)
948	21.20(7)	20.38(6)	19.53(6)	32.79(10)	23.96(7)	23.86(7)
963	20.37(6)	19.91(6)	19.10(6)	32.51(10)	23.86(7)	23.75(7)
977	19.54(6)	19.39(6)	18.64(5)	32.32(9)	23.85(7)	23.71(7)
991	18.71(5)	18.85(5)	18.16(5)	32.09(9)	23.79(7)	23.65(7)
1005	17.88(5)	18.28(5)	17.65(5)	31.90(9)	23.76(7)	23.60(7)
1019	17.11(5)	17.76(5)	17.18(5)	31.65(9)	23.68(7)	23.52(7)
1034	16.49(4)	17.37(5)	16.83(5)	31.37(9)	23.57(6)	23.40(6)
1048	15.99(4)	17.09(5)	16.58(4)	31.14(8)	23.51(6)	23.33(6)
1061	15.55(4)	16.87(4)	16.39(4)	30.93(8)	23.45(6)	23.26(6)
1076	15.15(4)	16.71(4)	16.26(4)	30.68(8)	23.36(6)	23.17(6)
1089	14.82(4)	16.59(4)	16.19(4)	30.47(8)	23.30(6)	23.10(6)
1103	14.53(4)	16.51(4)	16.15(4)	30.23(7)	23.23(6)	23.02(6)
1116	14.25(3)	16.41(4)	16.10(4)	30.03(7)	23.19(6)	22.98(6)
1130	13.96(3)	16.31(4)	16.03(4)	29.78(7)	23.08(6)	22.87(5)
1142	13.61(3)	16.14(4)	15.88(4)	29.64(7)	23.09(5)	22.88(5)
1156	13.19(3)	15.88(4)	15.66(4)	29.40(7)	23.00(5)	22.78(5)
1169	12.75(3)	15.57(4)	15.39(4)	29.22(7)	22.97(5)	22.75(5)
1181	12.32(3)	15.26(3)	15.13(3)	29.04(7)	22.92(5)	22.71(5)
1195	12.01(3)	15.06(3)	14.98(3)	28.79(6)	22.82(5)	22.60(5)
1207	11.83(3)	14.98(3)	14.94(3)	28.60(6)	22.74(5)	22.53(5)
1220	11.67(3)	14.88(3)	14.86(3)	28.45(6)	22.75(5)	22.55(5)
1233	11.51(2)	14.73(3)	14.70(3)	28.25(6)	22.68(5)	22.48(5)
1245	11.44(2)	14.66(3)	14.63(3)	28.04(6)	22.59(5)	22.39(5)

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