**Technical Article**

**Temperature-dependent structural behaviour of samarium cobalt oxide**

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Supplementary information

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. (Å3) | dens. (g/cm3) |
| 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) |
| 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) |

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) |
| 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) |

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Temp. (K) | Sm\_beq (Å2) | Co\_beq (Å2) | O1\_beq (Å2) | O2\_beq (Å2) |
| 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) |
| 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) |

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) |
| 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) |

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) |
| 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) |