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Experimental: $Sr_{5.8}La_{4.4}Ti_{7.8}S_{24}O_4$ (UM145)

A shiny black crystal with dimensions 0.31 x 0.28 x 0.28 mm was placed on the Enraf-Nonius CAD-4 diffractometer. The diffractometer was controlled with a Digital Equipment Corporation MicroVAX II (MVII) computer and the automated Enraf-Nonius program Express (version 5.1). The crystals' final cell parameters and crystal orientation matrix were determined from 25 reflections in the range 39.3 < 2 < 42.1; these constants were confirmed with axial photographs. Data were collected [MoK] with /2 scans over the range 2.7 < < 27.5 with a scan width of (1.24+0.88tan) and a variable scan speed of 2.1 - 4.1min.$^{-1}$ with each scan recorded in 96 steps with the outermost 16 steps on each end of the scan being used for background measurement. Three nearly orthogonal standard reflections were monitored at 1 hour intervals of X-ray exposure with minor variations in intensity being observed; data were not corrected. Seven -scan reflections were collected over the range 5.2 < < 21.1; the absorption correction was applied with transmission factors ranging from 0.4835 - 0.9960; average correction 0.7218. Data were collected with the indices (after later transformation) hkl; resulting in the measurement of 1292 reflections.

Structural determination and Refinement:

All crystallographic calculations were performed on a PC with a 486 DX2/66 processor and 16Mb of extended memory. Data were corrected for Lorentz and polarization factors, absorption and reduced to observed structure-factor amplitudes using the program package NRCVAX[1]. The lack of systematic absences enabled the possibility of many space groups in both the higher symmetry Tetragonal system and lower symmetry Orthorhombic system. Data were now exported as F_o^2 and ($F_o^{2)}$ to the crystallographic program package SHELX[2]. The structure proved troublesome and was successfully determined, initially, in P222 (no. 16) of the orthorhombic class. The program MISSYM[1] examined the atomic positions and indicated the existence of a four-fold axis and an inversion center indicating the tetragonal system. The structure was now determined in P4/mmm (no. 123) and refined with SHELXL-93[2], F_o^2 and (F_o^2). Subsequent difference-Fourier maps revealed the location of six sulfur and one oxygen atoms. Refinement of the structure converged well and it was apparent several of the sites were site scrambled and composed of two partial occupancy atoms. Many possibilities were attempted and when the refinement converged it was found that the true charge of the system deviated from zero so several restraints, SUMP instructions, were now included to force the overall charge to zero. The structure was refined to convergence [/ 0.001] with R(F)=5.35%, wR(F^2)=11.113% and GOF=1.032 for all 693 unique reflections [R(F)=4.28%, wR(F^2)=10.39% for those 553 data with Fo > 4(Fo)]. A final difference-Fourier map possessed large peaks within 1A of the heavy atoms and || 1.78 eA^{-3}.

The function minimized during the full-matrix least-squares refinement was w(Fo^2-Fc^2) where w=1/[^{2}(Fo^2) + (0.0623*P)^2] and P=(max(Fo^2 ,0) + 2 * Fc^2)/3. An empirical correction for extinction was also applied to the data in the form (Fc^2,corr) = k[1 + 0.001 * x * Fc^2 * ^{3}/sin(2)]$^{(-1/4)}$ where k=0.27462 is the overall scale factor. The value determined for x was 0.0029(5).

References:

1. Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S., (1989) *J.Appl. Cryst.*, 22, 384-387

2. Sheldrick, G.M., (1990). Acta Cryst. A46, 467-473.

The following label conversion were performed to obtain a common numbering scheme in the manuscript for $Sr_{5.8}La_{4.4}Ti_{7.8}S_{24}O_4$.

Supplementary Material atom label	Manuscript atom label
Ti(5)	Ti(3)
Ti(3)	M(3)
Sr(3)	M(3)
Ti(2)	M(2)
Sr(2)	M(2)

Table 1. Crystal data and structure refinement for UM145.

Identification code	p55
Empirical formula	$Sr_{5.8}La_{4.4}Ti_{7.8}S_{24}O_4$
Formula weight	291.33
Temperature	153(2) K
Wavelength	.71073 A
Crystal system	Tetragonal
Space group	P4/mmm
Unit cell dimensions	a = 10.569(3) A alpha = 90 deg. b = 10.569(3) A beta = 90 deg. c = 8.516(4) A gamma = 90 deg.
Volume	951.4(5) A^3
Z	8
Density (calculated)	4.068 Mg/m^3
Absorption coefficient	1.449 mm^-1
F(000)	1060
Crystal size	0.31 x 0.28 x 0.28 mm
Theta range for data collection	2.73 to 27.48 deg.
Index ranges	0<=h<=13, 0<=k<=13, 0<=l<=11
Reflections collected	1284
Independent reflections	693 [R(int) = 0.1161]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	693 / 4 / 56
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1039 [553 data]
R indices (all data)	R1 = 0.0535, wR2 = 0.1111
Extinction coefficient	.0029(5)
Largest diff. peak and hole	1.782 and -1.594 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for UM145. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
La(1)	2957(1)	2957(1)	2317(1)	6(1)
Sr(1)	2957(1)	2957(1)	2317(1)	6(1)
Sr(2)	0	0	5000	12(1)
Ti(2)	0	0	5000	12(1)
Sr(3)	5000	0	5000	43(1)
Ti(3)	5000	0	5000	43(1)
Ti(1)	0	5000	0	6(1)
Ti(4)	5000	5000	5000	7(1)
Ti(5)	0	2023(2)	0	9(1)
S(1)	5000	5000	2268(6)	8(1)
S(2)	2311(3)	5000	0	5(1)
S(3)	0	3413(2)	2120(3)	9(1)
S(4)	7335(3)	5000	5000	12(1)
S(5)	0	0	1744(7)	14(1)
S(6)	1791(3)	1791(3)	5000	25(1)
O(1)	1830(7)	1830(7)	0	13(2)

Table 4. Bond lengths [A] and angles [deg] for UM145.

La(1)-O(1)	2.595(7)
La(1)-S(6)	2.873(3)
La(1)-S(2)#1	3.0042(12)
La(1)-S(2)	3.0042(12)
La(1)-S(1)	3.0546(10)
La(1)-S(4)#2	3.1590(10)
La(1)-S(4)#3	3.1590(10)
La(1)-S(3)#4	3.1665(9)
La(1)-S(3)	3.1665(9)
La(1)-Ti(4)	3.8142(11)
La(1)-Ti(5)	3.8255(12)
La(1)-Ti(5)#5	3.8255(12)
Sr(1)-O(1)	2.595(7)
Sr(1)-S(6)	2.873(3)
Sr(1)-S(2)#1	3.0042(12)
Sr(1)-S(2)	3.0042(12)
Sr(1)-S(1)	3.0546(10)
Sr(1)-S(4)#2	3.1590(10)
Sr(1)-S(4)#3	3.1590(10)
Sr(1)-S(3)#4	3.1665(9)
Sr(1)-S(3)	3.1665(9)
Sr(1)-Ti(4)	3.8142(11)
Sr(1)-Ti(5)	3.8255(12)
Sr(1)-Ti(5)#5	3.8255(12)
Sr(2)-S(6)	2.677(5)
Sr(2)-S(6)#6	2.677(5)
Sr(2)-S(6)#7	2.677(5)
Sr(2)-S(6)#8	2.677(5)
Sr(2)-S(5)#6	2.773(6)
Sr(2)-S(5)	2.773(6)
Ti(2)-S(6)	2.677(5)
Ti(2)-S(6)#6	2.677(5)
Ti(2)-S(6)#7	2.677(5)
Ti(2)-S(6)#8	2.677(5)
Ti(2)-S(5)#6	2.773(6)
Ti(2)-S(5)	2.773(6)
Sr(3)-S(4)#2	2.816(4)
Sr(3)-S(4)#9	2.816(4)
Sr(3)-S(3)#10	2.971(3)
Sr(3)-S(3)#4	2.971(3)
Sr(3)-S(3)#1	2.971(3)
Sr(3)-S(3)#7	2.971(3)
Ti(3)-S(4)#2	2.816(4)
Ti(3)-S(4)#9	2.816(4)
Ti(3)-S(3)#10	2.971(3)
Ti(3)-S(3)#4	2.971(3)
Ti(3)-S(3)#1	2.971(3)
Ti(3)-S(3)#7	2.971(3)
Ti(1)-S(2)	2.443(3)
Ti(1)-S(2)#11	2.443(3)
Ti(1)-S(3)#12	2.464(3)
Ti(1)-S(3)#13	2.464(3)
Ti(1)-S(3)	2.464(3)
Ti(1)-S(3)#11	2.464(3)
Ti(1)-Ti(5)#11	3.147(2)

Ti(1)-Ti(5)	3.147(2)
Ti(4)-S(1)#3	2.327(5)
Ti(4)-S(1)	2.327(5)
Ti(4)-S(4)	2.468(4)
Ti(4)-S(4)#2	2.468(4)
Ti(4)-S(4)#1	2.468(4)
Ti(4)-S(4)#3	2.468(4)
Ti(4)-La(1)#3	3.8142(11)
Ti(4)-Sr(1)#3	3.8142(11)
Ti(4)-La(1)#2	3.8142(11)
Ti(4)-La(1)#10	3.8142(11)
Ti(5)-O(1)#8	1.944(7)
Ti(5)-O(1)	1.944(7)
Ti(5)-S(3)	2.328(3)
Ti(5)-S(3)#13	2.328(3)
Ti(5)-S(5)#14	2.603(4)
Ti(5)-S(5)	2.603(4)
Ti(5)-Ti(5)#8	3.023(3)
Ti(5)-Ti(5)#5	3.023(3)
Ti(5)-La(1)#15	3.8255(12)
S(1)-Sr(1)#16	3.0546(10)
S(1)-La(1)#16	3.0546(10)
S(1)-Sr(1)#17	3.0546(10)
S(1)-La(1)#17	3.0546(10)
S(1)-Sr(1)#1	3.0546(10)
S(1)-La(1)#1	3.0546(10)
S(2)-Sr(1)#17	3.0042(12)
S(2)-La(1)#17	3.0042(12)
S(2)-Sr(1)#13	3.0042(12)
S(2)-La(1)#13	3.0042(12)
S(2)-La(1)#18	3.0042(12)
S(2)-Sr(1)#18	3.0042(12)
S(3)-Ti(3)#8	2.971(3)
S(3)-Sr(3)#8	2.971(3)
S(3)-Sr(1)#8	3.1665(9)
S(3)-La(1)#8	3.1665(9)
S(4)-Ti(3)#1	2.816(4)
S(4)-Sr(3)#1	2.816(4)
S(4)-La(1)#1	3.1590(10)
S(4)-Sr(1)#1	3.1590(10)
S(4)-La(1)#3	3.1590(10)
S(4)-Sr(1)#3	3.1590(10)
S(4)-La(1)#10	3.1590(10)
S(4)-Sr(1)#16	3.1590(10)
S(4)-Sr(1)#10	3.1590(10)
S(4)-La(1)#16	3.1590(10)
S(5)-Ti(5)#8	2.603(4)
S(5)-Ti(5)#14	2.603(4)
S(5)-Ti(5)#5	2.603(4)
S(6)-Sr(1)#19	2.873(3)
S(6)-La(1)#19	2.873(3)
O(1)-Ti(5)#5	1.944(7)
O(1)-La(1)#13	2.595(7)
O(1)-Sr(1)#13	2.595(7)

O(1)-La(1)-S(6)	102.2(2)
O(1)-La(1)-S(2)#1	74.10(14)
S(6)-La(1)-S(2)#1	137.16(6)

O(1)-La(1)-S(2)	74.10(14)
S(6)-La(1)-S(2)	137.16(6)
S(2)#1-La(1)-S(2)	83.98(10)
O(1)-La(1)-S(1)	129.7(2)
S(6)-La(1)-S(1)	128.11(13)
S(2)#1-La(1)-S(1)	69.10(8)
S(2)-La(1)-S(1)	69.10(8)
O(1)-La(1)-S(4)#2	144.99(8)
S(6)-La(1)-S(4)#2	71.11(7)
S(2)#1-La(1)-S(4)#2	87.79(3)
S(2)-La(1)-S(4)#2	134.48(8)
S(1)-La(1)-S(4)#2	66.15(10)
O(1)-La(1)-S(4)#3	144.99(8)
S(6)-La(1)-S(4)#3	71.11(7)
S(2)#1-La(1)-S(4)#3	134.48(8)
S(2)-La(1)-S(4)#3	87.79(3)
S(1)-La(1)-S(4)#3	66.15(10)
S(4)#2-La(1)-S(4)#3	67.08(11)
O(1)-La(1)-S(3)#4	64.95(10)
S(6)-La(1)-S(3)#4	71.61(6)
S(2)#1-La(1)-S(3)#4	68.37(7)
S(2)-La(1)-S(3)#4	135.17(5)
S(1)-La(1)-S(3)#4	126.10(5)
S(4)#2-La(1)-S(3)#4	80.66(8)
S(4)#3-La(1)-S(3)#4	136.72(5)
O(1)-La(1)-S(3)	64.95(10)
S(6)-La(1)-S(3)	71.61(6)
S(2)#1-La(1)-S(3)	135.17(5)
S(2)-La(1)-S(3)	68.37(7)
S(1)-La(1)-S(3)	126.10(5)
S(4)#2-La(1)-S(3)	136.72(5)
S(4)#3-La(1)-S(3)	80.66(8)
S(3)#4-La(1)-S(3)	107.34(9)
O(1)-La(1)-Ti(4)	167.3(2)
S(6)-La(1)-Ti(4)	90.53(9)
S(2)#1-La(1)-Ti(4)	96.61(4)
S(2)-La(1)-Ti(4)	96.61(4)
S(1)-La(1)-Ti(4)	37.58(10)
S(4)#2-La(1)-Ti(4)	40.09(7)
S(4)#3-La(1)-Ti(4)	40.09(7)
S(3)#4-La(1)-Ti(4)	120.28(5)
S(3)-La(1)-Ti(4)	120.28(5)
O(1)-La(1)-Ti(5)	27.64(10)
S(6)-La(1)-Ti(5)	87.09(8)
S(2)#1-La(1)-Ti(5)	100.94(4)
S(2)-La(1)-Ti(5)	70.19(6)
S(1)-La(1)-Ti(5)	138.84(9)
S(4)#2-La(1)-Ti(5)	155.01(6)
S(4)#3-La(1)-Ti(5)	118.01(7)
S(3)#4-La(1)-Ti(5)	80.94(6)
S(3)-La(1)-Ti(5)	37.42(5)
Ti(4)-La(1)-Ti(5)	156.58(3)
O(1)-La(1)-Ti(5)#5	27.64(10)
S(6)-La(1)-Ti(5)#5	87.09(8)
S(2)#1-La(1)-Ti(5)#5	70.19(6)
S(2)-La(1)-Ti(5)#5	100.94(4)
S(1)-La(1)-Ti(5)#5	138.84(9)
S(4)#2-La(1)-Ti(5)#5	118.01(7)

S(4)#3-La(1)-Ti(5)#5	155.01(6)
S(3)#4-La(1)-Ti(5)#5	37.42(5)
S(3)-La(1)-Ti(5)#5	80.94(6)
Ti(4)-La(1)-Ti(5)#5	156.58(3)
Ti(5)-La(1)-Ti(5)#5	46.55(6)
O(1)-Sr(1)-S(6)	102.2(2)
O(1)-Sr(1)-S(2)#1	74.10(14)
S(6)-Sr(1)-S(2)#1	137.16(6)
O(1)-Sr(1)-S(2)	74.10(14)
S(6)-Sr(1)-S(2)	137.16(6)
S(2)#1-Sr(1)-S(2)	83.98(10)
O(1)-Sr(1)-S(1)	129.7(2)
S(6)-Sr(1)-S(1)	128.11(13)
S(2)#1-Sr(1)-S(1)	69.10(8)
S(2)-Sr(1)-S(1)	69.10(8)
O(1)-Sr(1)-S(4)#2	144.99(8)
S(6)-Sr(1)-S(4)#2	71.11(7)
S(2)#1-Sr(1)-S(4)#2	87.79(3)
S(2)-Sr(1)-S(4)#2	134.48(8)
S(1)-Sr(1)-S(4)#2	66.15(10)
O(1)-Sr(1)-S(4)#3	144.99(8)
S(6)-Sr(1)-S(4)#3	71.11(7)
S(2)#1-Sr(1)-S(4)#3	134.48(8)
S(2)-Sr(1)-S(4)#3	87.79(3)
S(1)-Sr(1)-S(4)#3	66.15(10)
S(4)#2-Sr(1)-S(4)#3	67.08(11)
O(1)-Sr(1)-S(3)#4	64.95(10)
S(6)-Sr(1)-S(3)#4	71.61(6)
S(2)#1-Sr(1)-S(3)#4	68.37(7)
S(2)-Sr(1)-S(3)#4	135.17(5)
S(1)-Sr(1)-S(3)#4	126.10(5)
S(4)#2-Sr(1)-S(3)#4	80.66(8)
S(4)#3-Sr(1)-S(3)#4	136.72(5)
O(1)-Sr(1)-S(3)	64.95(10)
S(6)-Sr(1)-S(3)	71.61(6)
S(2)#1-Sr(1)-S(3)	135.17(5)
S(2)-Sr(1)-S(3)	68.37(7)
S(1)-Sr(1)-S(3)	126.10(5)
S(4)#2-Sr(1)-S(3)	136.72(5)
S(4)#3-Sr(1)-S(3)	80.66(8)
S(3)#4-Sr(1)-S(3)	107.34(9)
O(1)-Sr(1)-Ti(4)	167.3(2)
S(6)-Sr(1)-Ti(4)	90.53(9)
S(2)#1-Sr(1)-Ti(4)	96.61(4)
S(2)-Sr(1)-Ti(4)	96.61(4)
S(1)-Sr(1)-Ti(4)	37.58(10)
S(4)#2-Sr(1)-Ti(4)	40.09(7)
S(4)#3-Sr(1)-Ti(4)	40.09(7)
S(3)#4-Sr(1)-Ti(4)	120.28(5)
S(3)-Sr(1)-Ti(4)	120.28(5)
O(1)-Sr(1)-Ti(5)	27.64(10)
S(6)-Sr(1)-Ti(5)	87.09(8)
S(2)#1-Sr(1)-Ti(5)	100.94(4)
S(2)-Sr(1)-Ti(5)	70.19(6)
S(1)-Sr(1)-Ti(5)	138.84(9)
S(4)#2-Sr(1)-Ti(5)	155.01(6)
S(4)#3-Sr(1)-Ti(5)	118.01(7)
S(3)#4-Sr(1)-Ti(5)	80.94(6)

S(3)-Sr(1)-Ti(5)	37.42(5)
Ti(4)-Sr(1)-Ti(5)	156.58(3)
O(1)-Sr(1)-Ti(5)#5	27.64(10)
S(6)-Sr(1)-Ti(5)#5	87.09(8)
S(2)#1-Sr(1)-Ti(5)#5	70.19(6)
S(2)-Sr(1)-Ti(5)#5	100.94(4)
S(1)-Sr(1)-Ti(5)#5	138.84(9)
S(4)#2-Sr(1)-Ti(5)#5	118.01(7)
S(4)#3-Sr(1)-Ti(5)#5	155.01(6)
S(3)#4-Sr(1)-Ti(5)#5	37.42(5)
S(3)-Sr(1)-Ti(5)#5	80.94(6)
Ti(4)-Sr(1)-Ti(5)#5	156.58(3)
Ti(5)-Sr(1)-Ti(5)#5	46.55(6)
S(6)-Sr(2)-S(6)#6	180.0
S(6)-Sr(2)-S(6)#7	90.0
S(6)#6-Sr(2)-S(6)#7	90.0
S(6)-Sr(2)-S(6)#8	90.0
S(6)#6-Sr(2)-S(6)#8	90.0
S(6)#7-Sr(2)-S(6)#8	180.0
S(6)-Sr(2)-S(5)#6	90.0
S(6)#6-Sr(2)-S(5)#6	90.0
S(6)#7-Sr(2)-S(5)#6	90.0
S(6)#8-Sr(2)-S(5)#6	90.0
S(6)-Sr(2)-S(5)	90.0
S(6)#6-Sr(2)-S(5)	90.0
S(6)#7-Sr(2)-S(5)	90.0
S(6)#8-Sr(2)-S(5)	90.0
S(5)#6-Sr(2)-S(5)	180.0
S(6)-Ti(2)-S(6)#6	180.0
S(6)-Ti(2)-S(6)#7	90.0
S(6)#6-Ti(2)-S(6)#7	90.0
S(6)-Ti(2)-S(6)#8	90.0
S(6)#6-Ti(2)-S(6)#8	90.0
S(6)#7-Ti(2)-S(6)#8	180.0
S(6)-Ti(2)-S(5)#6	90.0
S(6)#6-Ti(2)-S(5)#6	90.0
S(6)#7-Ti(2)-S(5)#6	90.0
S(6)#8-Ti(2)-S(5)#6	90.0
S(6)-Ti(2)-S(5)	90.0
S(6)#6-Ti(2)-S(5)	90.0
S(6)#7-Ti(2)-S(5)	90.0
S(6)#8-Ti(2)-S(5)	90.0
S(5)#6-Ti(2)-S(5)	180.0
S(4)#2-Sr(3)-S(4)#9	180.0
S(4)#2-Sr(3)-S(3)#10	90.0
S(4)#9-Sr(3)-S(3)#10	90.0
S(4)#2-Sr(3)-S(3)#4	90.0
S(4)#9-Sr(3)-S(3)#4	90.0
S(3)#10-Sr(3)-S(3)#4	180.0
S(4)#2-Sr(3)-S(3)#1	90.0
S(4)#9-Sr(3)-S(3)#1	90.0
S(3)#10-Sr(3)-S(3)#1	111.28(10)
S(3)#4-Sr(3)-S(3)#1	68.72(10)
S(4)#2-Sr(3)-S(3)#7	90.0
S(4)#9-Sr(3)-S(3)#7	90.0
S(3)#10-Sr(3)-S(3)#7	68.72(10)
S(3)#4-Sr(3)-S(3)#7	111.28(10)
S(3)#1-Sr(3)-S(3)#7	180.0

S(4)#2-Ti(3)-S(4)#9	180.0
S(4)#2-Ti(3)-S(3)#10	90.0
S(4)#9-Ti(3)-S(3)#10	90.0
S(4)#2-Ti(3)-S(3)#4	90.0
S(4)#9-Ti(3)-S(3)#4	90.0
S(3)#10-Ti(3)-S(3)#4	180.0
S(4)#2-Ti(3)-S(3)#1	90.0
S(4)#9-Ti(3)-S(3)#1	90.0
S(3)#10-Ti(3)-S(3)#1	111.28(10)
S(3)#4-Ti(3)-S(3)#1	68.72(10)
S(4)#2-Ti(3)-S(3)#7	90.0
S(4)#9-Ti(3)-S(3)#7	90.0
S(3)#10-Ti(3)-S(3)#7	68.72(10)
S(3)#4-Ti(3)-S(3)#7	111.28(10)
S(3)#1-Ti(3)-S(3)#7	180.0
S(2)-Ti(1)-S(2)#11	180.0
S(2)-Ti(1)-S(3)#12	90.0
S(2)#11-Ti(1)-S(3)#12	90.0
S(2)-Ti(1)-S(3)#13	90.0
S(2)#11-Ti(1)-S(3)#13	90.0
S(3)#12-Ti(1)-S(3)#13	180.0
S(2)-Ti(1)-S(3)	90.0
S(2)#11-Ti(1)-S(3)	90.0
S(3)#12-Ti(1)-S(3)	85.77(13)
S(3)#13-Ti(1)-S(3)	94.23(13)
S(2)-Ti(1)-S(3)#11	90.0
S(2)#11-Ti(1)-S(3)#11	90.0
S(3)#12-Ti(1)-S(3)#11	94.23(13)
S(3)#13-Ti(1)-S(3)#11	85.77(13)
S(3)-Ti(1)-S(3)#11	180.0
S(2)-Ti(1)-Ti(5)#11	90.0
S(2)#11-Ti(1)-Ti(5)#11	90.0
S(3)#12-Ti(1)-Ti(5)#11	47.11(6)
S(3)#13-Ti(1)-Ti(5)#11	132.89(6)
S(3)-Ti(1)-Ti(5)#11	132.89(6)
S(3)#11-Ti(1)-Ti(5)#11	47.11(6)
S(2)-Ti(1)-Ti(5)	90.0
S(2)#11-Ti(1)-Ti(5)	90.0
S(3)#12-Ti(1)-Ti(5)	132.89(6)
S(3)#13-Ti(1)-Ti(5)	47.11(6)
S(3)-Ti(1)-Ti(5)	47.11(6)
S(3)#11-Ti(1)-Ti(5)	132.89(6)
Ti(5)#11-Ti(1)-Ti(5)	180.0
S(1)#3-Ti(4)-S(1)	180.0
S(1)#3-Ti(4)-S(4)	90.0
S(1)-Ti(4)-S(4)	90.0
S(1)#3-Ti(4)-S(4)#2	90.0
S(1)-Ti(4)-S(4)#2	90.0
S(4)-Ti(4)-S(4)#2	90.0
S(1)#3-Ti(4)-S(4)#1	90.0
S(1)-Ti(4)-S(4)#1	90.0
S(4)-Ti(4)-S(4)#1	90.0
S(4)#2-Ti(4)-S(4)#1	180.0
S(1)#3-Ti(4)-S(4)#3	90.0
S(1)-Ti(4)-S(4)#3	90.0
S(4)-Ti(4)-S(4)#3	180.0
S(4)#2-Ti(4)-S(4)#3	90.0
S(4)#1-Ti(4)-S(4)#3	90.0

S(1)#3-Ti(4)-La(1)#3	53.20(2)
S(1)-Ti(4)-La(1)#3	126.80(2)
S(4)-Ti(4)-La(1)#3	55.512(9)
S(4)#2-Ti(4)-La(1)#3	124.488(9)
S(4)#1-Ti(4)-La(1)#3	55.512(9)
S(4)#3-Ti(4)-La(1)#3	124.488(9)
S(1)#3-Ti(4)-Sr(1)#3	53.20(2)
S(1)-Ti(4)-Sr(1)#3	126.80(2)
S(4)-Ti(4)-Sr(1)#3	55.512(9)
S(4)#2-Ti(4)-Sr(1)#3	124.488(9)
S(4)#1-Ti(4)-Sr(1)#3	55.512(9)
S(4)#3-Ti(4)-Sr(1)#3	124.488(9)
La(1)#3-Ti(4)-Sr(1)#3	.00(3)
S(1)#3-Ti(4)-Sr(1)	126.80(2)
S(1)-Ti(4)-Sr(1)	53.20(2)
S(4)-Ti(4)-Sr(1)	124.488(9)
S(4)#2-Ti(4)-Sr(1)	55.512(9)
S(4)#1-Ti(4)-Sr(1)	124.488(9)
S(4)#3-Ti(4)-Sr(1)	55.512(9)
La(1)#3-Ti(4)-Sr(1)	180.0
Sr(1)#3-Ti(4)-Sr(1)	180.0
S(1)#3-Ti(4)-La(1)	126.80(2)
S(1)-Ti(4)-La(1)	53.20(2)
S(4)-Ti(4)-La(1)	124.488(9)
S(4)#2-Ti(4)-La(1)	55.512(9)
S(4)#1-Ti(4)-La(1)	124.488(9)
S(4)#3-Ti(4)-La(1)	55.512(9)
La(1)#3-Ti(4)-La(1)	180.0
Sr(1)#3-Ti(4)-La(1)	180.0
Sr(1)-Ti(4)-La(1)	.00(3)
S(1)#3-Ti(4)-La(1)#2	53.20(2)
S(1)-Ti(4)-La(1)#2	126.80(2)
S(4)-Ti(4)-La(1)#2	124.488(9)
S(4)#2-Ti(4)-La(1)#2	124.488(9)
S(4)#1-Ti(4)-La(1)#2	55.512(9)
S(4)#3-Ti(4)-La(1)#2	55.512(9)
La(1)#3-Ti(4)-La(1)#2	68.98(2)
Sr(1)#3-Ti(4)-La(1)#2	68.98(2)
Sr(1)-Ti(4)-La(1)#2	111.02(2)
La(1)-Ti(4)-La(1)#2	111.02(2)
S(1)#3-Ti(4)-La(1)#10	53.20(2)
S(1)-Ti(4)-La(1)#10	126.80(2)
S(4)-Ti(4)-La(1)#10	55.512(9)
S(4)#2-Ti(4)-La(1)#10	55.512(9)
S(4)#1-Ti(4)-La(1)#10	124.488(9)
S(4)#3-Ti(4)-La(1)#10	124.488(9)
La(1)#3-Ti(4)-La(1)#10	68.98(2)
Sr(1)#3-Ti(4)-La(1)#10	68.98(2)
Sr(1)-Ti(4)-La(1)#10	111.02(2)
La(1)-Ti(4)-La(1)#10	111.02(2)
La(1)#2-Ti(4)-La(1)#10	106.41(3)
O(1)#8-Ti(5)-O(1)	167.9(5)
O(1)#8-Ti(5)-S(3)	93.8(2)
O(1)-Ti(5)-S(3)	93.8(2)
O(1)#8-Ti(5)-S(3)#13	93.8(2)
O(1)-Ti(5)-S(3)#13	93.8(2)
S(3)-Ti(5)-S(3)#13	101.7(2)
O(1)#8-Ti(5)-S(5)#14	85.1(2)

O(1)-Ti(5)-S(5)#14	85.1(2)
S(3)-Ti(5)-S(5)#14	163.9(2)
S(3)#13-Ti(5)-S(5)#14	94.37(13)
O(1)#8-Ti(5)-S(5)	85.1(2)
O(1)-Ti(5)-S(5)	85.1(2)
S(3)-Ti(5)-S(5)	94.37(13)
S(3)#13-Ti(5)-S(5)	163.9(2)
S(5)#14-Ti(5)-S(5)	69.6(2)
O(1)#8-Ti(5)-Ti(5)#8	39.0(3)
O(1)-Ti(5)-Ti(5)#8	129.0(3)
S(3)-Ti(5)-Ti(5)#8	116.52(5)
S(3)#13-Ti(5)-Ti(5)#8	116.52(5)
S(5)#14-Ti(5)-Ti(5)#8	54.50(6)
S(5)-Ti(5)-Ti(5)#8	54.50(6)
O(1)#8-Ti(5)-Ti(5)#5	129.0(3)
O(1)-Ti(5)-Ti(5)#5	39.0(3)
S(3)-Ti(5)-Ti(5)#5	116.52(5)
S(3)#13-Ti(5)-Ti(5)#5	116.52(5)
S(5)#14-Ti(5)-Ti(5)#5	54.50(6)
S(5)-Ti(5)-Ti(5)#5	54.50(6)
Ti(5)#8-Ti(5)-Ti(5)#5	90.0
O(1)#8-Ti(5)-Ti(1)	96.0(3)
O(1)-Ti(5)-Ti(1)	96.0(3)
S(3)-Ti(5)-Ti(1)	50.85(8)
S(3)#13-Ti(5)-Ti(1)	50.85(8)
S(5)#14-Ti(5)-Ti(1)	145.21(12)
S(5)-Ti(5)-Ti(1)	145.21(12)
Ti(5)#8-Ti(5)-Ti(1)	135.0
Ti(5)#5-Ti(5)-Ti(1)	135.0
O(1)#8-Ti(5)-La(1)	147.08(9)
O(1)-Ti(5)-La(1)	38.25(14)
S(3)-Ti(5)-La(1)	55.74(2)
S(3)#13-Ti(5)-La(1)	103.72(6)
S(5)#14-Ti(5)-La(1)	120.41(5)
S(5)-Ti(5)-La(1)	85.27(7)
Ti(5)#8-Ti(5)-La(1)	139.47(3)
Ti(5)#5-Ti(5)-La(1)	66.72(3)
Ti(1)-Ti(5)-La(1)	75.05(3)
O(1)#8-Ti(5)-Sr(1)	147.08(9)
O(1)-Ti(5)-Sr(1)	38.25(14)
S(3)-Ti(5)-Sr(1)	55.74(2)
S(3)#13-Ti(5)-Sr(1)	103.72(6)
S(5)#14-Ti(5)-Sr(1)	120.41(5)
S(5)-Ti(5)-Sr(1)	85.27(7)
Ti(5)#8-Ti(5)-Sr(1)	139.47(3)
Ti(5)#5-Ti(5)-Sr(1)	66.72(3)
Ti(1)-Ti(5)-Sr(1)	75.05(3)
La(1)-Ti(5)-Sr(1)	.00(3)
O(1)#8-Ti(5)-La(1)#15	38.25(14)
O(1)-Ti(5)-La(1)#15	147.08(9)
S(3)-Ti(5)-La(1)#15	103.72(6)
S(3)#13-Ti(5)-La(1)#15	55.74(2)
S(5)#14-Ti(5)-La(1)#15	85.27(7)
S(5)-Ti(5)-La(1)#15	120.41(5)
Ti(5)#8-Ti(5)-La(1)#15	66.72(3)
Ti(5)#5-Ti(5)-La(1)#15	139.47(3)
Ti(1)-Ti(5)-La(1)#15	75.05(3)
La(1)-Ti(5)-La(1)#15	150.09(7)

Sr(1)-Ti(5)-La(1)#15	150.09(7)
Ti(4)-S(1)-Sr(1)#16	89.21(10)
Ti(4)-S(1)-La(1)#16	89.21(10)
Sr(1)#16-S(1)-La(1)#16	.00(4)
Ti(4)-S(1)-Sr(1)	89.21(10)
Sr(1)#16-S(1)-Sr(1)	178.4(2)
La(1)#16-S(1)-Sr(1)	178.4(2)
Ti(4)-S(1)-La(1)	89.21(10)
Sr(1)#16-S(1)-La(1)	178.4(2)
La(1)#16-S(1)-La(1)	178.4(2)
Sr(1)-S(1)-La(1)	.00(4)
Ti(4)-S(1)-Sr(1)#17	89.21(10)
Sr(1)#16-S(1)-Sr(1)#17	89.989(3)
La(1)#16-S(1)-Sr(1)#17	89.989(3)
Sr(1)-S(1)-Sr(1)#17	89.989(3)
La(1)-S(1)-Sr(1)#17	89.989(3)
Ti(4)-S(1)-La(1)#17	89.21(10)
Sr(1)#16-S(1)-La(1)#17	89.989(3)
La(1)#16-S(1)-La(1)#17	89.989(3)
Sr(1)-S(1)-La(1)#17	89.989(3)
La(1)-S(1)-La(1)#17	89.989(3)
Sr(1)#17-S(1)-La(1)#17	.00(3)
Ti(4)-S(1)-Sr(1)#1	89.21(10)
Sr(1)#16-S(1)-Sr(1)#1	89.989(3)
La(1)#16-S(1)-Sr(1)#1	89.989(3)
Sr(1)-S(1)-Sr(1)#1	89.989(3)
La(1)-S(1)-Sr(1)#1	89.989(3)
Sr(1)#17-S(1)-Sr(1)#1	178.4(2)
La(1)#17-S(1)-Sr(1)#1	178.4(2)
Ti(4)-S(1)-La(1)#1	89.21(10)
Sr(1)#16-S(1)-La(1)#1	89.989(3)
La(1)#16-S(1)-La(1)#1	89.989(3)
Sr(1)-S(1)-La(1)#1	89.989(3)
La(1)-S(1)-La(1)#1	89.989(3)
Sr(1)#17-S(1)-La(1)#1	178.4(2)
La(1)#17-S(1)-La(1)#1	178.4(2)
Sr(1)#1-S(1)-La(1)#1	.00(3)
Ti(1)-S(2)-Sr(1)#17	103.13(6)
Ti(1)-S(2)-La(1)#17	103.13(6)
Sr(1)#17-S(2)-La(1)#17	.00(2)
Ti(1)-S(2)-Sr(1)#13	103.13(6)
Sr(1)#17-S(2)-Sr(1)#13	153.74(12)
La(1)#17-S(2)-Sr(1)#13	153.74(12)
Ti(1)-S(2)-La(1)#13	103.13(6)
Sr(1)#17-S(2)-La(1)#13	153.74(12)
La(1)#17-S(2)-La(1)#13	153.74(12)
Sr(1)#13-S(2)-La(1)#13	.00(4)
Ti(1)-S(2)-La(1)#18	103.13(6)
Sr(1)#17-S(2)-La(1)#18	82.13(4)
La(1)#17-S(2)-La(1)#18	82.13(4)
Sr(1)#13-S(2)-La(1)#18	91.93(5)
La(1)#13-S(2)-La(1)#18	91.93(5)
Ti(1)-S(2)-Sr(1)#18	103.13(6)
Sr(1)#17-S(2)-Sr(1)#18	82.13(4)
La(1)#17-S(2)-Sr(1)#18	82.13(4)
Sr(1)#13-S(2)-Sr(1)#18	91.93(5)
La(1)#13-S(2)-Sr(1)#18	91.93(5)
La(1)#18-S(2)-Sr(1)#18	.00(2)

Ti(1)-S(2)-Sr(1)	103.13(6)
Sr(1)#17-S(2)-Sr(1)	91.93(5)
La(1)#17-S(2)-Sr(1)	91.93(5)
Sr(1)#13-S(2)-Sr(1)	82.13(4)
La(1)#13-S(2)-Sr(1)	82.13(4)
La(1)#18-S(2)-Sr(1)	153.74(12)
Sr(1)#18-S(2)-Sr(1)	153.74(12)
Ti(1)-S(2)-La(1)	103.13(6)
Sr(1)#17-S(2)-La(1)	91.93(5)
La(1)#17-S(2)-La(1)	91.93(5)
Sr(1)#13-S(2)-La(1)	82.13(4)
La(1)#13-S(2)-La(1)	82.13(4)
La(1)#18-S(2)-La(1)	153.74(12)
Sr(1)#18-S(2)-La(1)	153.74(12)
Sr(1)-S(2)-La(1)	.00(4)
Ti(5)-S(3)-Ti(1)	82.04(10)
Ti(5)-S(3)-Ti(3)#8	175.21(12)
Ti(1)-S(3)-Ti(3)#8	102.75(9)
Ti(5)-S(3)-Sr(3)#8	175.21(12)
Ti(1)-S(3)-Sr(3)#8	102.75(9)
Ti(3)#8-S(3)-Sr(3)#8	.0
Ti(5)-S(3)-Sr(1)#8	86.84(5)
Ti(1)-S(3)-Sr(1)#8	98.20(4)
Ti(3)#8-S(3)-Sr(1)#8	92.42(5)
Sr(3)#8-S(3)-Sr(1)#8	92.42(5)
Ti(5)-S(3)-La(1)#8	86.84(5)
Ti(1)-S(3)-La(1)#8	98.20(4)
Ti(3)#8-S(3)-La(1)#8	92.42(5)
Sr(3)#8-S(3)-La(1)#8	92.42(5)
Sr(1)#8-S(3)-La(1)#8	.00(3)
Ti(5)-S(3)-Sr(1)	86.84(5)
Ti(1)-S(3)-Sr(1)	98.20(4)
Ti(3)#8-S(3)-Sr(1)	92.42(5)
Sr(3)#8-S(3)-Sr(1)	92.42(5)
Sr(1)#8-S(3)-Sr(1)	161.42(9)
La(1)#8-S(3)-Sr(1)	161.42(9)
Ti(5)-S(3)-La(1)	86.84(5)
Ti(1)-S(3)-La(1)	98.20(4)
Ti(3)#8-S(3)-La(1)	92.42(5)
Sr(3)#8-S(3)-La(1)	92.42(5)
Sr(1)#8-S(3)-La(1)	161.42(9)
La(1)#8-S(3)-La(1)	161.42(9)
Sr(1)-S(3)-La(1)	.00(3)
Ti(4)-S(4)-Ti(3)#1	180.0
Ti(4)-S(4)-Sr(3)#1	180.0
Ti(3)#1-S(4)-Sr(3)#1	.0
Ti(4)-S(4)-La(1)#1	84.39(7)
Ti(3)#1-S(4)-La(1)#1	95.61(7)
Sr(3)#1-S(4)-La(1)#1	95.61(7)
Ti(4)-S(4)-Sr(1)#1	84.39(7)
Ti(3)#1-S(4)-Sr(1)#1	95.61(7)
Sr(3)#1-S(4)-Sr(1)#1	95.61(7)
La(1)#1-S(4)-Sr(1)#1	.00(2)
Ti(4)-S(4)-La(1)#3	84.39(7)
Ti(3)#1-S(4)-La(1)#3	95.61(7)
Sr(3)#1-S(4)-La(1)#3	95.61(7)
La(1)#1-S(4)-La(1)#3	168.79(13)
Sr(1)#1-S(4)-La(1)#3	168.79(13)

Ti(4)-S(4)-Sr(1)#3	84.39(7)
Ti(3)#1-S(4)-Sr(1)#3	95.61(7)
Sr(3)#1-S(4)-Sr(1)#3	95.61(7)
La(1)#1-S(4)-Sr(1)#3	168.79(13)
Sr(1)#1-S(4)-Sr(1)#3	168.79(13)
La(1)#3-S(4)-Sr(1)#3	.00(3)
Ti(4)-S(4)-La(1)#10	84.39(7)
Ti(3)#1-S(4)-La(1)#10	95.61(7)
Sr(3)#1-S(4)-La(1)#10	95.61(7)
La(1)#1-S(4)-La(1)#10	92.64(4)
Sr(1)#1-S(4)-La(1)#10	92.64(4)
La(1)#3-S(4)-La(1)#10	86.26(4)
Sr(1)#3-S(4)-La(1)#10	86.26(4)
Ti(4)-S(4)-Sr(1)#16	84.39(7)
Ti(3)#1-S(4)-Sr(1)#16	95.61(7)
Sr(3)#1-S(4)-Sr(1)#16	95.61(7)
La(1)#1-S(4)-Sr(1)#16	86.26(4)
Sr(1)#1-S(4)-Sr(1)#16	86.26(4)
La(1)#3-S(4)-Sr(1)#16	92.64(4)
Sr(1)#3-S(4)-Sr(1)#16	92.64(4)
La(1)#10-S(4)-Sr(1)#16	168.79(13)
Ti(4)-S(4)-Sr(1)#10	84.39(7)
Ti(3)#1-S(4)-Sr(1)#10	95.61(7)
Sr(3)#1-S(4)-Sr(1)#10	95.61(7)
La(1)#1-S(4)-Sr(1)#10	92.64(4)
Sr(1)#1-S(4)-Sr(1)#10	92.64(4)
La(1)#3-S(4)-Sr(1)#10	86.26(4)
Sr(1)#3-S(4)-Sr(1)#10	86.26(4)
La(1)#10-S(4)-Sr(1)#10	.00(2)
Sr(1)#16-S(4)-Sr(1)#10	168.79(13)
Ti(4)-S(4)-La(1)#16	84.39(7)
Ti(3)#1-S(4)-La(1)#16	95.61(7)
Sr(3)#1-S(4)-La(1)#16	95.61(7)
La(1)#1-S(4)-La(1)#16	86.26(4)
Sr(1)#1-S(4)-La(1)#16	86.26(4)
La(1)#3-S(4)-La(1)#16	92.64(4)
Sr(1)#3-S(4)-La(1)#16	92.64(4)
La(1)#10-S(4)-La(1)#16	168.79(13)
Sr(1)#16-S(4)-La(1)#16	.00(3)
Sr(1)#10-S(4)-La(1)#16	168.79(13)
Ti(5)#8-S(5)-Ti(5)#14	71.01(12)
Ti(5)#8-S(5)-Ti(5)	71.01(12)
Ti(5)#14-S(5)-Ti(5)	110.4(2)
Ti(5)#8-S(5)-Ti(5)#5	110.4(2)
Ti(5)#14-S(5)-Ti(5)#5	71.01(12)
Ti(5)-S(5)-Ti(5)#5	71.01(12)
Ti(5)#8-S(5)-Ti(2)	124.79(12)
Ti(5)#14-S(5)-Ti(2)	124.79(12)
Ti(5)-S(5)-Ti(2)	124.79(12)
Ti(5)#5-S(5)-Ti(2)	124.79(12)
Ti(5)#8-S(5)-Sr(2)	124.79(12)
Ti(5)#14-S(5)-Sr(2)	124.79(12)
Ti(5)-S(5)-Sr(2)	124.79(12)
Ti(5)#5-S(5)-Sr(2)	124.79(12)
Ti(2)-S(5)-Sr(2)	.0
Ti(2)-S(6)-Sr(2)	.0
Ti(2)-S(6)-Sr(1)#19	127.33(8)
Sr(2)-S(6)-Sr(1)#19	127.33(8)

Ti(2)-S(6)-La(1)#19	127.33(8)
Sr(2)-S(6)-La(1)#19	127.33(8)
Sr(1)#19-S(6)-La(1)#19	.00(4)
Ti(2)-S(6)-Sr(1)	127.33(8)
Sr(2)-S(6)-Sr(1)	127.33(8)
Sr(1)#19-S(6)-Sr(1)	105.3(2)
La(1)#19-S(6)-Sr(1)	105.3(2)
Ti(2)-S(6)-La(1)	127.33(8)
Sr(2)-S(6)-La(1)	127.33(8)
Sr(1)#19-S(6)-La(1)	105.3(2)
La(1)#19-S(6)-La(1)	105.3(2)
Sr(1)-S(6)-La(1)	.00(4)
Ti(5)#5-O(1)-Ti(5)	102.1(5)
Ti(5)#5-O(1)-La(1)	114.10(6)
Ti(5)-O(1)-La(1)	114.10(6)
Ti(5)#5-O(1)-Sr(1)	114.10(6)
Ti(5)-O(1)-Sr(1)	114.10(6)
La(1)-O(1)-Sr(1)	.00(4)
Ti(5)#5-O(1)-La(1)#13	114.10(6)
Ti(5)-O(1)-La(1)#13	114.10(6)
La(1)-O(1)-La(1)#13	99.0(4)
Sr(1)-O(1)-La(1)#13	99.0(4)
Ti(5)#5-O(1)-Sr(1)#13	114.10(6)
Ti(5)-O(1)-Sr(1)#13	114.10(6)
La(1)-O(1)-Sr(1)#13	99.0(4)
Sr(1)-O(1)-Sr(1)#13	99.0(4)
La(1)#13-O(1)-Sr(1)#13	.00(4)

Symmetry transformations used to generate equivalent atoms:
#1 -y+1,x,z #2 y,-x+1,-z+1 #3 -x+1,-y+1,-z+1
#4 y,-x,z #5 y,-x,-z #6 -x,-y,-z+1
#7 y,-x,-z+1 #8 -y,x,z #9 -y+1,x-1,z
#10 -y+1,x,-z+1 #11 -x,-y+1,-z #12 -x,-y+1,z
#13 x,y,-z #14 -x,-y,-z #15 -y,x,-z
#16 -x+1,-y+1,z #17 y,-x+1,z #18 y,-x+1,-z
#19 x,y,-z+1

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for UM145. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
La(1)	5(1)	5(1)	8(1)	-1(1)	-1(1)	0(1)
Sr(1)	5(1)	5(1)	8(1)	-1(1)	-1(1)	0(1)
Sr(2)	13(1)	13(1)	10(2)	0	0	0
Ti(2)	13(1)	13(1)	10(2)	0	0	0
Sr(3)	123(3)	2(1)	3(1)	0	0	0
Ti(3)	123(3)	2(1)	3(1)	0	0	0
Ti(1)	5(2)	6(2)	7(2)	0	0	0
Ti(4)	7(2)	7(2)	7(2)	0	0	0
Ti(5)	5(1)	4(1)	19(1)	0	0	0
S(1)	6(1)	6(1)	11(3)	0	0	0
S(2)	4(2)	3(2)	9(2)	0	0	0
S(3)	8(1)	7(1)	11(1)	5(1)	0	0
S(4)	4(2)	13(2)	19(2)	0	0	0
S(5)	5(1)	5(1)	31(3)	0	0	0
S(6)	35(2)	35(2)	4(2)	0	0	-6(2)
O(1)	8(3)	8(3)	24(6)	0	0	4(4)

Rietveld .rie file for $Sr_{5.8}La_{4.4}Ti_{7.8}S_{24}O_4$ (UM145)

```
   1   1   0   7   0   0   0   0
   1   0   1   1   1   1   1   1   1   1   0   0
   2   4   6
   6   6   6
 0.00000 0.00000  0.0000 15.0000  0.0000 10.0000  0.0200 58.0000
  0.3000  1.0000  1.0000  1.0000  1.0000
   0      0.14858 0.00000
             0.00    0.00
 1.99707e+03 1.59005e+02 5.13873e+00 7.08686e-02 3.64770e-04-5.96611e+03
    0.00         0.00         0.00         0.00         0.00         0.00
   15.41   16.30
   19.27   20.15
   27.51   28.27
   31.07   31.52
   33.66   34.05
   35.53   36.02
   46.00   46.43
   1   1   1   1   1   1   1
UM145
P 4/m m m              6                  4.16190
  16   0   0   0   0   5   0   0   0   0
O1      O-2    0          0.20686 0.20686 0.00000 0.05000 1.00000
                             0.00    0.00    0.00    0.00    0.00
                          0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                             0.00    0.00    0.00    0.00    0.00    0.00
S6      S-2    0          0.16500 0.16500 0.50000 0.05000 1.00000
                             0.00    0.00    0.00    0.00    0.00
                          0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
```

			0.00	0.00	0.00	0.00	0.00	0.00	
S5	S-2	0	0.00000	0.00000	0.19071	0.05000	1.00000		
			0.00	0.00	0.00	0.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
S4	S-2	0	0.74407	0.50000	0.50000	0.05000	1.00000		
			0.00	0.00	0.00	0.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
S3	S-2	0	0.00000	0.34493	0.21036	0.27240	1.00000		
			0.00	0.00	0.00	51.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
S2	S-2	0	0.21665	0.50000	0.00000	4.14670	1.00000		
			0.00	0.00	0.00	61.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
S1	S-2	0	0.50000	0.50000	0.23373	0.05000	1.00000		
			0.00	0.00	0.00	0.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
Ti5	Ti+4	0	0.00000	0.21308	0.00000	0.05000	1.00000		
			0.00	0.00	0.00	0.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	
Ti4	Ti+4	0	0.50000	0.50000	0.50000	4.63927	1.00000		
			0.00	0.00	0.00	31.00	0.00		
			0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
			0.00	0.00	0.00	0.00	0.00	0.00	

```
Ti1     Ti+4   0        0.00000 0.50000 0.0000012.43071 1.00000
                           0.00    0.00    0.00   41.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
Ti3     Ti+4   0        0.50000 0.00000 0.5000012.62725 0.16500
                           0.00    0.00    0.00   11.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
Sr3     Sr+2   0        0.50000 0.00000 0.5000012.62725 0.83500
                           0.00    0.00    0.00   11.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
Ti2     Ti+4   0        0.00000 0.00000 0.50000 0.34827 0.42500
                           0.00    0.00    0.00   21.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
Sr2     Sr+2   0        0.00000 0.00000 0.50000 0.34827 0.57500
                           0.00    0.00    0.00   21.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
Sr1     Sr+2   0        0.29340 0.29340 0.23978 0.05000 0.44200
                           0.00    0.00    0.00    0.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
La1     La+3   0        0.29340 0.29340 0.23978 0.05000 0.55800
                           0.00    0.00    0.00    0.00    0.00
                        0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                           0.00    0.00    0.00    0.00    0.00    0.00
45.92510  0.0000  0.0000
```

```
 0.00     0.00     0.00
3    30.0000000.0000004.664696-.0605490.000000
                  0.00     0.00     0.00     0.00
                       4.542943-.0679350.000000
                           0.00     0.00     0.00
0     1.394244-1.18928.28739220.0000000.0000000.0000000.0000000.0000000.000000
          0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
0     .0477966-.096921.04265590.0000000.0000000.0000000.0000000.0000000.000000
          0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00     0.00
10.5081310.50813 8.42426 90.0000 90.0000 90.0000
 0.00     0.00     0.00     0.00     0.00     0.00
2    0  0.0000   0.0000   1.0000   0.9508   0.0000
                                     0.00     0.00
```


Experimental: $La_{14}Ti_8S_{33}O_4$ (UM178)

A shiny black capped pyramid shaped crystal with dimensions 0.1250 x 0.10 x 0.025 mm was placed on the Enraf-Nonius CAD-4 diffractometer. The crystals' final cell parameters and crystal orientation matrix were determined from 25 reflections in the range 17.6 < < 22.0; these constants were confirmed with axial photographs. Data were collected [MoK] with /2 scans over the range 2.0 - 25.0 with a scan width of (0.38+0.64tan) and a variable scan speed of 2.3 - 3.3min.$^{-1}$ with each scan recorded in 96 steps with the outermost 16 steps on each end of the scan being used for background measurement. The diffractometer was controlled with a Digital Equipment Corporation MicroVAX II (MVII) computer and the Enraf-Nonius VAX\VMS CAD4 control program. Three nearly orthogonal standard reflections were monitored at 1 hour intervals of X-ray exposure. Minimal variations in intensity, up to 4% for a single standard, were observed; data were not corrected. Nine -scan reflections were collected over the range 9.1 < < 21.3 resulting in a max:min transmission correction of 0.2914:0.1434. Data were collected with the indices hk-l; resulting in the measurement of 4594 reflections; 2287 unique [R(int)=0.0515].

Structural determination and Refinement:

All crystallographic calculations were performed on a PC with a 486 DX2/66 processor and 16Mb of extended memory. Data were corrected for Lorentz and polarization factors and reduced to F_o^2 and (F_o^2) using the program XCAD4[1]. The SHELXTL[2] program package was now implemented to determine the space group and apply the empirical absorption correction. The original data were collected for a triclinic cell[3] but several cell reduction programs[4] indicated the true crystal system to be monoclinic C-centered; later confirmed with axial photo's. Systematic absences indicated the monoclinic centrosymmetric space group C 2/m (no.12) or the non-centrosymmetric space groups C2 (no. 5) or Cm (no. 8). Intensity statistics favored the centrosymmetric possibility and it was in this space group, C2/m, that the structure was successfully determined. Structural determinations were attempted using XS[2] in all three monoclinic space groups but a solution was not to be found. The system was now returned to its initial triclinic state from whence the structure was successfully determined with the location of seven Lanthanum atoms (two later found to be partially occupied by Strontium) and five Titanium atoms. SHELXL[3] was now used to refine the structure, based upon F_o^2 and (F_o^2). The remaining atoms were determined using two cycles of a cyclic refinement-difference-Fourier map procedure. It was now quite obvious from the atomic positions that extra crystallographic symmetry was present in the form of a perpendicular mirror plane through 0,0,0 and an inversion center at -0.5,-0.5,-0.5[5]. The structure and reflections were now transformed to the monoclinic setting using the program XTRANS[6] and the atom list was now scrutinized for duplicates. The atom list was now reduced to five fully occupied lanthanum atoms and one sulfur atom, S(11), found to lie approximately 0.995A from itself. This atom was refined as a half-occupancy sulfur[7] while two of the other sulfur atoms were also found to have partially occupied sites. All atoms were refined anisotropically and the structure was refined to convergence [/ 0.001] with R(F)=5.20%, wR(F^2)=10.75% and GOF=1.094 for all 2286 unique reflections [R(F)=3.92%, wR(F^2)=10.00% for those 1880 data with Fo > 4(Fo)].

A final difference-Fourier map possessed several large peaks within 1A of the heavier lanthanum atoms with || 1.97 eA^{-3}; the remainder of the map was essentially featureless.

The function minimized during the full-matrix least-squares refinement was $w(Fo^2-Fc^2)$ where $w=1/[^2(Fo^2) + (0.0517*P)^2 + 40.71*P]$ and $P=(max(Fo^2,0) + 2 * Fc^2)/3$. An empirical correction for extinction (x) was also applied to the data in the form $(Fc^2,corr) = k[1 + 0.001 * x * Fc^2 * ^3/sin(2)]^{(-1/4)}$ where k=0.03132 is the overall scale factor. The value determined for x was 0.00063(4).

References:

1. Harms, K., (1993)

2. Sheldrick, G.M., (1990). *Acta Cryst.* A46, 467-473.

3. The data collection program, Enraf-Nonius' EXPRESS, chose the lower symmetry triclinic cell for data collection.

4a. DIRAX Duisenberg, A.J.M., *J.Appl. Cryst.* (1992), 25, 92-96.
4b. CREDUC, NRCVAX program package, Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S., *J.Appl. Cryst.* (1989) , **22**, 384-387)
4c. XPREP, SHELXTL program package, Siemens Industrial Automation Inc., Sheldrick, G.M.

5. MISSYM, NRCVAX program package, Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S., *J.Appl. Cryst.* (1989) , **22**, 384-387)

6. XTRANS (Doedens, Ziller, 1994?)

7. The structure was initially determined in the space group P-1 (no.2) with this same sulfur atom showing disorder (partial occupancy over two sites) and found to lie an equivalent distance from itself. Refinement of the ensemble in P-1 converged well with 'duplicate' positions as described *vide infra*.

The following label conversion were performed to obtain a common numbering scheme in the manuscript for $La_{14}Ti_8S_{33}O_4$.

Supplementary Material atom label	Manuscript atom label
S(5)	S(7)
S(7)	S(2)
S(2)	S(5)
S(1)	S(3)
S(3)	S(1)

Table 1. Crystal data and structure refinement for UM178.

Identification code	i
Empirical formula	La7 O2 S16.50 Ti4
Formula weight	1724.96
Temperature	153(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	C2/m
Unit cell dimensions	a = 14.9037(6) A alpha = 90 deg. b = 14.7355(11) A beta = 112.773(5) deg c = 12.2777(10) A gamma = 90 deg.
Volume, Z	2486.2(3) A^3, 4
Density (calculated)	4.608 Mg/m^3
Absorption coefficient	14.333 mm^-1
F(000)	3068
Crystal size	0.125 x 0.100 x 0.025 mm
Theta range for data collection	2.03 to 25.02 deg.
Limiting indices	-16<=h<=17, -17<=k<=17, -14<=l<=0
Reflections collected	4594
Independent reflections	2287 [R(int) = 0.0515]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.2916 and 0.1437
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2286 / 0 / 156
Goodness-of-fit on F^2	1.094
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1000 [1880 Data]
R indices (all data)	R1 = 0.0520, wR2 = 0.1075
Extinction coefficient	0.00063(4)
Largest diff. peak and hole	1.974 and -2.674 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for UM178. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
La(1)	4457(1)	7907(1)	8268(1)	9(1)
La(2)	3460(1)	10000	11797(1)	8(1)
La(3)	2408(1)	10000	8337(1)	9(1)
La(4)	3679(1)	5000	5534(1)	18(1)
La(5)	3421(1)	8010(1)	4317(1)	24(1)
Ti(1)	2500	7500	10000	10(1)
Ti(2)	3921(2)	10000	6446(3)	14(1)
Ti(3)	6012(1)	6010(1)	10004(2)	8(1)
S(1)	3802(2)	6705(2)	11606(2)	10(1)
S(2)	4583(3)	5000	8637(3)	9(1)
S(3)	4553(3)	10000	8440(3)	9(1)
S(4)	2258(2)	8289(2)	11645(2)	9(1)
S(5)	2714(2)	8847(2)	6491(3)	15(1)
S(6)	3161(3)	10000	4180(4)	11(1)
S(7)	3667(2)	8671(2)	10010(2)	9(1)
S(8)	5064(2)	8770(2)	6481(2)	10(1)
S(9)	3618(2)	6808(2)	6225(3)	23(1)
S(10)	0	1631(6)	5000	12(2)
S(11)	680(4)	9679(4)	6352(5)	13(1)
O(1)	5000	6860(7)	10000	8(2)
O(2)	1875(7)	10000	10040(9)	7(2)

Table 3. Bond lengths [A] and angles [deg] for UM178.

La(1)-O(1)	2.494(7)
La(1)-S(9)	2.837(3)
La(1)-S(8)	2.964(3)
La(1)-S(7)#1	2.997(3)
La(1)-S(5)	3.007(3)
La(1)-S(7)	3.030(3)
La(1)-S(3)	3.0916(8)
La(1)-S(1)#1	3.094(3)
La(1)-S(4)#2	3.141(3)
La(1)-Ti(2)	3.712(2)
La(1)-Ti(3)	3.728(2)
La(1)-Ti(3)#1	3.734(2)
La(2)-O(2)	2.508(10)
La(2)-S(8)#3	2.998(3)
La(2)-S(8)#1	2.998(3)
La(2)-S(7)	3.044(3)
La(2)-S(7)#4	3.044(3)
La(2)-S(4)	3.056(3)
La(2)-S(4)#4	3.056(3)
La(2)-S(3)#3	3.085(4)
La(2)-S(6)#5	3.127(4)
La(2)-Ti(2)#3	3.656(3)
La(2)-Ti(3)#6	3.763(2)
La(2)-Ti(3)#7	3.763(2)
La(3)-O(2)	2.508(10)
La(3)-S(11)	2.818(5)
La(3)-S(11)#4	2.818(5)
La(3)-S(7)#4	2.930(3)
La(3)-S(7)	2.930(3)
La(3)-S(5)	3.005(3)
La(3)-S(5)#4	3.005(3)
La(3)-S(1)#2	3.110(3)
La(3)-S(1)#8	3.110(3)
La(3)-S(3)	3.149(4)
La(3)-Ti(3)#6	3.747(2)
La(3)-Ti(3)#7	3.747(2)
La(4)-S(11)#9	2.794(5)
La(4)-S(11)#10	2.794(5)
La(4)-S(9)	2.808(3)
La(4)-S(9)#11	2.808(3)
La(4)-S(11)#12	2.866(5)
La(4)-S(11)#13	2.866(5)
La(4)-S(6)#13	2.896(4)
La(4)-S(5)#12	3.063(3)
La(4)-S(5)#13	3.063(3)
La(4)-S(10)#14	3.329(6)
La(4)-S(10)#15	3.329(6)
La(4)-Ti(2)#13	3.692(3)
La(5)-S(9)	2.860(3)
La(5)-S(9)#13	2.860(4)
La(5)-S(6)	2.9542(10)
La(5)-S(10)#14	2.973(6)
La(5)-S(8)#16	3.004(3)
La(5)-S(8)	3.046(3)

La(5)-S(4)#17	3.088(3)
La(5)-S(5)#13	3.167(3)
La(5)-Ti(2)	3.805(2)
La(5)-La(5)#13	4.021(2)
Ti(1)-S(7)#2	2.447(3)
Ti(1)-S(7)	2.447(3)
Ti(1)-S(1)#2	2.463(3)
Ti(1)-S(1)	2.463(3)
Ti(1)-S(4)#2	2.474(3)
Ti(1)-S(4)	2.474(3)
Ti(1)-Ti(3)#1	3.122(2)
Ti(1)-Ti(3)#6	3.122(2)
Ti(2)-S(3)	2.258(5)
Ti(2)-S(8)#4	2.476(3)
Ti(2)-S(8)	2.476(3)
Ti(2)-S(5)	2.491(3)
Ti(2)-S(5)#4	2.491(3)
Ti(2)-S(6)	2.565(5)
Ti(2)-La(2)#3	3.656(3)
Ti(2)-La(4)#13	3.692(3)
Ti(2)-La(1)#4	3.712(2)
Ti(2)-La(5)#4	3.805(2)
Ti(3)-O(2)#10	1.957(6)
Ti(3)-O(1)	1.959(7)
Ti(3)-S(1)#1	2.337(3)
Ti(3)-S(4)#9	2.383(3)
Ti(3)-S(2)	2.608(4)
Ti(3)-S(2)#18	2.632(3)
Ti(3)-Ti(3)#11	2.976(4)
Ti(3)-Ti(3)#1	3.012(3)
Ti(3)-Ti(1)#1	3.122(2)
Ti(3)-La(1)#1	3.734(2)
Ti(3)-La(3)#10	3.747(2)
S(1)-Ti(3)#1	2.337(3)
S(1)-La(1)#1	3.094(3)
S(1)-La(3)#2	3.110(3)
S(2)-Ti(3)#11	2.608(4)
S(2)-Ti(3)#18	2.632(3)
S(2)-Ti(3)#1	2.632(3)
S(3)-La(2)#3	3.085(4)
S(3)-La(1)#4	3.0916(7)
S(4)-Ti(3)#6	2.383(3)
S(4)-La(5)#5	3.088(3)
S(4)-La(1)#2	3.141(3)
S(5)-La(4)#13	3.063(3)
S(5)-La(5)#13	3.167(3)
S(6)-La(4)#13	2.896(4)
S(6)-La(5)#4	2.9542(10)
S(6)-La(2)#17	3.127(4)
S(7)-La(1)#1	2.997(3)
S(8)-La(2)#3	2.998(3)
S(8)-La(5)#16	3.004(3)
S(9)-La(5)#13	2.860(3)
S(10)-S(11)#19	2.492(9)
S(10)-S(11)#11	2.492(9)
S(10)-La(5)#12	2.973(6)
S(10)-La(5)#20	2.973(6)
S(10)-La(4)#20	3.329(6)

S(10)-La(4)#15	3.329(6)
S(11)-S(11)#4	0.946(12)
S(11)-S(10)#19	2.492(9)
S(11)-La(4)#7	2.794(5)
S(11)-La(4)#13	2.866(5)
O(1)-Ti(3)#1	1.959(7)
O(1)-La(1)#1	2.494(7)
O(2)-Ti(3)#6	1.957(6)
O(2)-Ti(3)#7	1.957(6)

O(1)-La(1)-S(9)	106.7(2)
O(1)-La(1)-S(8)	143.63(6)
S(9)-La(1)-S(8)	75.36(8)
O(1)-La(1)-S(7)#1	74.0(2)
S(9)-La(1)-S(7)#1	144.11(9)
S(8)-La(1)-S(7)#1	83.81(7)
O(1)-La(1)-S(5)	143.84(6)
S(9)-La(1)-S(5)	70.11(9)
S(8)-La(1)-S(5)	71.98(8)
S(7)#1-La(1)-S(5)	130.30(8)
O(1)-La(1)-S(7)	73.4(2)
S(9)-La(1)-S(7)	132.63(9)
S(8)-La(1)-S(7)	132.53(8)
S(7)#1-La(1)-S(7)	82.75(8)
S(5)-La(1)-S(7)	82.99(8)
O(1)-La(1)-S(3)	124.6(2)
S(9)-La(1)-S(3)	128.51(10)
S(8)-La(1)-S(3)	66.60(9)
S(7)#1-La(1)-S(3)	64.59(9)
S(5)-La(1)-S(3)	66.04(9)
S(7)-La(1)-S(3)	66.48(8)
O(1)-La(1)-S(1)#1	67.35(10)
S(9)-La(1)-S(1)#1	77.99(9)
S(8)-La(1)-S(1)#1	78.03(7)
S(7)#1-La(1)-S(1)#1	69.20(7)
S(5)-La(1)-S(1)#1	140.52(8)
S(7)-La(1)-S(1)#1	136.47(7)
S(3)-La(1)-S(1)#1	123.50(9)
O(1)-La(1)-S(4)#2	67.90(10)
S(9)-La(1)-S(4)#2	67.90(8)
S(8)-La(1)-S(4)#2	138.75(7)
S(7)#1-La(1)-S(4)#2	137.41(7)
S(5)-La(1)-S(4)#2	78.29(8)
S(7)-La(1)-S(4)#2	68.92(7)
S(3)-La(1)-S(4)#2	125.02(8)
S(1)#1-La(1)-S(4)#2	110.80(7)
O(1)-La(1)-Ti(2)	161.9(2)
S(9)-La(1)-Ti(2)	91.31(8)
S(8)-La(1)-Ti(2)	41.69(7)
S(7)#1-La(1)-Ti(2)	92.14(7)
S(5)-La(1)-Ti(2)	41.90(7)
S(7)-La(1)-Ti(2)	93.70(7)
S(3)-La(1)-Ti(2)	37.38(8)
S(1)#1-La(1)-Ti(2)	119.10(7)
S(4)#2-La(1)-Ti(2)	119.90(7)
O(1)-La(1)-Ti(3)	28.90(11)
S(9)-La(1)-Ti(3)	92.38(8)
S(8)-La(1)-Ti(3)	116.42(6)

S(7)#1-La(1)-Ti(3)	71.03(6)
S(5)-La(1)-Ti(3)	158.66(7)
S(7)-La(1)-Ti(3)	101.57(6)
S(3)-La(1)-Ti(3)	134.99(8)
S(1)#1-La(1)-Ti(3)	38.67(6)
S(4)#2-La(1)-Ti(3)	83.91(6)
Ti(2)-La(1)-Ti(3)	155.35(5)
O(1)-La(1)-Ti(3)#1	28.77(11)
S(9)-La(1)-Ti(3)#1	87.69(7)
S(8)-La(1)-Ti(3)#1	156.86(6)
S(7)#1-La(1)-Ti(3)#1	102.08(6)
S(5)-La(1)-Ti(3)#1	117.25(6)
S(7)-La(1)-Ti(3)#1	70.61(6)
S(3)-La(1)-Ti(3)#1	136.19(8)
S(1)#1-La(1)-Ti(3)#1	83.17(6)
S(4)#2-La(1)-Ti(3)#1	39.38(6)
Ti(2)-La(1)-Ti(3)#1	156.98(5)
Ti(3)-La(1)-Ti(3)#1	47.61(5)
O(2)-La(2)-S(8)#3	142.76(5)
O(2)-La(2)-S(8)#1	142.76(6)
S(8)#3-La(2)-S(8)#1	74.37(11)
O(2)-La(2)-S(7)	72.8(2)
S(8)#3-La(2)-S(7)	130.25(7)
S(8)#1-La(2)-S(7)	82.44(7)
O(2)-La(2)-S(7)#4	72.8(2)
S(8)#3-La(2)-S(7)#4	82.44(7)
S(8)#1-La(2)-S(7)#4	130.25(7)
S(7)-La(2)-S(7)#4	80.08(10)
O(2)-La(2)-S(4)	67.21(11)
S(8)#3-La(2)-S(4)	142.57(8)
S(8)#1-La(2)-S(4)	78.29(7)
S(7)-La(2)-S(4)	69.25(7)
S(7)#4-La(2)-S(4)	134.99(8)
O(2)-La(2)-S(4)#4	67.21(11)
S(8)#3-La(2)-S(4)#4	78.29(7)
S(8)#1-La(2)-S(4)#4	142.57(8)
S(7)-La(2)-S(4)#4	134.99(8)
S(7)#4-La(2)-S(4)#4	69.25(7)
S(4)-La(2)-S(4)#4	111.15(10)
O(2)-La(2)-S(3)#3	122.5(2)
S(8)#3-La(2)-S(3)#3	66.29(7)
S(8)#1-La(2)-S(3)#3	66.29(7)
S(7)-La(2)-S(3)#3	64.13(7)
S(7)#4-La(2)-S(3)#3	64.13(7)
S(4)-La(2)-S(3)#3	123.74(5)
S(4)#4-La(2)-S(3)#3	123.74(5)
O(2)-La(2)-S(6)#5	112.1(2)
S(8)#3-La(2)-S(6)#5	70.81(8)
S(8)#1-La(2)-S(6)#5	70.81(7)
S(7)-La(2)-S(6)#5	139.96(5)
S(7)#4-La(2)-S(6)#5	139.96(5)
S(4)-La(2)-S(6)#5	76.38(6)
S(4)#4-La(2)-S(6)#5	76.38(6)
S(3)#3-La(2)-S(6)#5	125.32(10)
O(2)-La(2)-Ti(2)#3	160.5(2)
S(8)#3-La(2)-Ti(2)#3	42.26(5)
S(8)#1-La(2)-Ti(2)#3	42.26(6)
S(7)-La(2)-Ti(2)#3	92.46(6)

S(7)#4-La(2)-Ti(2)#3	92.46(6)
S(4)-La(2)-Ti(2)#3	120.17(5)
S(4)#4-La(2)-Ti(2)#3	120.17(5)
S(3)#3-La(2)-Ti(2)#3	37.96(9)
S(6)#5-La(2)-Ti(2)#3	87.37(9)
O(2)-La(2)-Ti(3)#6	28.29(13)
S(8)#3-La(2)-Ti(3)#6	158.74(6)
S(8)#1-La(2)-Ti(3)#6	116.99(6)
S(7)-La(2)-Ti(3)#6	70.71(6)
S(7)#4-La(2)-Ti(3)#6	100.29(6)
S(4)-La(2)-Ti(3)#6	39.21(6)
S(4)#4-La(2)-Ti(3)#6	82.97(6)
S(3)#3-La(2)-Ti(3)#6	133.93(7)
S(6)#5-La(2)-Ti(3)#6	95.15(7)
Ti(2)#3-La(2)-Ti(3)#6	156.52(3)
O(2)-La(2)-Ti(3)#7	28.29(13)
S(8)#3-La(2)-Ti(3)#7	116.99(6)
S(8)#1-La(2)-Ti(3)#7	158.74(6)
S(7)-La(2)-Ti(3)#7	100.29(6)
S(7)#4-La(2)-Ti(3)#7	70.71(6)
S(4)-La(2)-Ti(3)#7	82.97(6)
S(4)#4-La(2)-Ti(3)#7	39.21(6)
S(3)#3-La(2)-Ti(3)#7	133.93(7)
S(6)#5-La(2)-Ti(3)#7	95.15(7)
Ti(2)#3-La(2)-Ti(3)#7	156.52(3)
Ti(3)#6-La(2)-Ti(3)#7	46.60(6)
O(2)-La(3)-S(11)	104.0(2)
O(2)-La(3)-S(11)#4	104.0(2)
S(11)-La(3)-S(11)#4	19.3(2)
O(2)-La(3)-S(7)#4	74.9(2)
S(11)-La(3)-S(7)#4	147.26(13)
S(11)#4-La(3)-S(7)#4	128.09(13)
O(2)-La(3)-S(7)	74.9(2)
S(11)-La(3)-S(7)	128.09(13)
S(11)#4-La(3)-S(7)	147.26(13)
S(7)#4-La(3)-S(7)	83.86(11)
O(2)-La(3)-S(5)	144.91(7)
S(11)-La(3)-S(5)	66.90(12)
S(11)#4-La(3)-S(5)	78.31(12)
S(7)#4-La(3)-S(5)	131.58(8)
S(7)-La(3)-S(5)	84.72(8)
O(2)-La(3)-S(5)#4	144.91(7)
S(11)-La(3)-S(5)#4	78.31(12)
S(11)#4-La(3)-S(5)#4	66.90(12)
S(7)#4-La(3)-S(5)#4	84.72(8)
S(7)-La(3)-S(5)#4	131.58(8)
S(5)-La(3)-S(5)#4	68.87(12)
O(2)-La(3)-S(1)#2	66.88(12)
S(11)-La(3)-S(1)#2	62.59(12)
S(11)#4-La(3)-S(1)#2	79.10(13)
S(7)#4-La(3)-S(1)#2	138.03(8)
S(7)-La(3)-S(1)#2	70.35(7)
S(5)-La(3)-S(1)#2	79.56(8)
S(5)#4-La(3)-S(1)#2	137.10(8)
O(2)-La(3)-S(1)#8	66.88(11)
S(11)-La(3)-S(1)#8	79.10(13)
S(11)#4-La(3)-S(1)#8	62.59(12)
S(7)#4-La(3)-S(1)#8	70.35(7)

S(7)-La(3)-S(1)#8	138.03(8)
S(5)-La(3)-S(1)#8	137.10(8)
S(5)#4-La(3)-S(1)#8	79.56(7)
S(1)#2-La(3)-S(1)#8	107.79(10)
O(2)-La(3)-S(3)	127.6(2)
S(11)-La(3)-S(3)	127.50(13)
S(11)#4-La(3)-S(3)	127.50(13)
S(7)#4-La(3)-S(3)	66.89(7)
S(7)-La(3)-S(3)	66.89(7)
S(5)-La(3)-S(3)	65.33(8)
S(5)#4-La(3)-S(3)	65.33(8)
S(1)#2-La(3)-S(3)	126.00(5)
S(1)#8-La(3)-S(3)	126.00(5)
O(2)-La(3)-Ti(3)#6	28.61(13)
S(11)-La(3)-Ti(3)#6	83.72(11)
S(11)#4-La(3)-Ti(3)#6	91.37(11)
S(7)#4-La(3)-Ti(3)#6	102.86(6)
S(7)-La(3)-Ti(3)#6	72.05(6)
S(5)-La(3)-Ti(3)#6	117.77(6)
S(5)#4-La(3)-Ti(3)#6	156.23(7)
S(1)#2-La(3)-Ti(3)#6	38.45(6)
S(1)#8-La(3)-Ti(3)#6	81.88(6)
S(3)-La(3)-Ti(3)#6	138.40(7)
O(2)-La(3)-Ti(3)#7	28.61(12)
S(11)-La(3)-Ti(3)#7	91.37(11)
S(11)#4-La(3)-Ti(3)#7	83.72(11)
S(7)#4-La(3)-Ti(3)#7	72.05(6)
S(7)-La(3)-Ti(3)#7	102.86(6)
S(5)-La(3)-Ti(3)#7	156.23(7)
S(5)#4-La(3)-Ti(3)#7	117.77(6)
S(1)#2-La(3)-Ti(3)#7	81.88(6)
S(1)#8-La(3)-Ti(3)#7	38.45(6)
S(3)-La(3)-Ti(3)#7	138.40(7)
Ti(3)#6-La(3)-Ti(3)#7	46.81(6)
S(11)#9-La(4)-S(11)#10	19.5(2)
S(11)#9-La(4)-S(9)	83.45(13)
S(11)#10-La(4)-S(9)	101.95(14)
S(11)#9-La(4)-S(9)#11	101.95(14)
S(11)#10-La(4)-S(9)#11	83.45(13)
S(9)-La(4)-S(9)#11	143.15(14)
S(11)#9-La(4)-S(11)#12	71.0(2)
S(11)#10-La(4)-S(11)#12	67.6(2)
S(9)-La(4)-S(11)#12	117.43(14)
S(9)#11-La(4)-S(11)#12	98.48(14)
S(11)#9-La(4)-S(11)#13	67.6(2)
S(11)#10-La(4)-S(11)#13	71.0(2)
S(9)-La(4)-S(11)#13	98.48(14)
S(9)#11-La(4)-S(11)#13	117.43(14)
S(11)#12-La(4)-S(11)#13	19.0(2)
S(11)#9-La(4)-S(6)#13	152.30(13)
S(11)#10-La(4)-S(6)#13	152.30(13)
S(9)-La(4)-S(6)#13	79.65(7)
S(9)#11-La(4)-S(6)#13	79.65(7)
S(11)#12-La(4)-S(6)#13	136.50(13)
S(11)#13-La(4)-S(6)#13	136.50(13)
S(11)#9-La(4)-S(5)#12	132.80(12)
S(11)#10-La(4)-S(5)#12	119.45(13)
S(9)-La(4)-S(5)#12	132.87(9)

S(9)#11-La(4)-S(5)#12	68.14(8)
S(11)#12-La(4)-S(5)#12	65.54(12)
S(11)#13-La(4)-S(5)#12	76.64(13)
S(6)#13-La(4)-S(5)#12	73.87(9)
S(11)#9-La(4)-S(5)#13	119.45(13)
S(11)#10-La(4)-S(5)#13	132.80(12)
S(9)-La(4)-S(5)#13	68.14(8)
S(9)#11-La(4)-S(5)#13	132.87(9)
S(11)#12-La(4)-S(5)#13	76.64(13)
S(11)#13-La(4)-S(5)#13	65.54(12)
S(6)#13-La(4)-S(5)#13	73.87(9)
S(5)#12-La(4)-S(5)#13	67.39(11)
S(11)#9-La(4)-S(10)#14	47.03(14)
S(11)#10-La(4)-S(10)#14	64.07(14)
S(9)-La(4)-S(10)#14	57.68(12)
S(9)#11-La(4)-S(10)#14	146.66(12)
S(11)#12-La(4)-S(10)#14	63.41(14)
S(11)#13-La(4)-S(10)#14	46.69(13)
S(6)#13-La(4)-S(10)#14	133.13(10)
S(5)#12-La(4)-S(10)#14	120.49(7)
S(5)#13-La(4)-S(10)#14	72.92(7)
S(11)#9-La(4)-S(10)#15	64.07(14)
S(11)#10-La(4)-S(10)#15	47.03(14)
S(9)-La(4)-S(10)#15	146.66(12)
S(9)#11-La(4)-S(10)#15	57.68(12)
S(11)#12-La(4)-S(10)#15	46.69(13)
S(11)#13-La(4)-S(10)#15	63.41(14)
S(6)#13-La(4)-S(10)#15	133.13(10)
S(5)#12-La(4)-S(10)#15	72.92(7)
S(5)#13-La(4)-S(10)#15	120.49(7)
S(10)#14-La(4)-S(10)#15	92.5(2)
S(11)#9-La(4)-Ti(2)#13	159.84(12)
S(11)#10-La(4)-Ti(2)#13	159.84(12)
S(9)-La(4)-Ti(2)#13	92.88(7)
S(9)#11-La(4)-Ti(2)#13	92.88(7)
S(11)#12-La(4)-Ti(2)#13	93.51(11)
S(11)#13-La(4)-Ti(2)#13	93.51(11)
S(6)#13-La(4)-Ti(2)#13	43.78(9)
S(5)#12-La(4)-Ti(2)#13	41.99(6)
S(5)#13-La(4)-Ti(2)#13	41.99(6)
S(10)#14-La(4)-Ti(2)#13	114.85(6)
S(10)#15-La(4)-Ti(2)#13	114.85(6)
S(9)-La(5)-S(9)#13	90.67(9)
S(9)-La(5)-S(6)	129.13(11)
S(9)#13-La(5)-S(6)	77.84(10)
S(9)-La(5)-S(10)#14	61.76(9)
S(9)#13-La(5)-S(10)#14	141.57(14)
S(6)-La(5)-S(10)#14	140.03(14)
S(9)-La(5)-S(8)#16	130.29(9)
S(9)#13-La(5)-S(8)#16	138.91(9)
S(6)-La(5)-S(8)#16	73.14(9)
S(10)#14-La(5)-S(8)#16	74.58(11)
S(9)-La(5)-S(8)	73.78(8)
S(9)#13-La(5)-S(8)	126.27(8)
S(6)-La(5)-S(8)	74.22(9)
S(10)#14-La(5)-S(8)	73.97(11)
S(8)#16-La(5)-S(8)	72.27(9)
S(9)-La(5)-S(4)#17	142.20(8)

S(9)#13-La(5)-S(4)#17	68.39(8)
S(6)-La(5)-S(4)#17	78.46(10)
S(10)#14-La(5)-S(4)#17	116.61(6)
S(8)#16-La(5)-S(4)#17	77.70(7)
S(8)-La(5)-S(4)#17	143.99(8)
S(9)-La(5)-S(5)#13	66.07(8)
S(9)#13-La(5)-S(5)#13	67.53(9)
S(6)-La(5)-S(5)#13	142.86(9)
S(10)#14-La(5)-S(5)#13	76.51(13)
S(8)#16-La(5)-S(5)#13	126.70(8)
S(8)-La(5)-S(5)#13	137.96(8)
S(4)#17-La(5)-S(5)#13	76.72(8)
S(9)-La(5)-Ti(2)	89.10(8)
S(9)#13-La(5)-Ti(2)	89.74(8)
S(6)-La(5)-Ti(2)	42.32(8)
S(10)#14-La(5)-Ti(2)	114.19(10)
S(8)#16-La(5)-Ti(2)	87.97(7)
S(8)-La(5)-Ti(2)	40.51(6)
S(4)#17-La(5)-Ti(2)	120.48(7)
S(5)#13-La(5)-Ti(2)	145.06(7)
S(9)-La(5)-La(5)#13	45.34(7)
S(9)#13-La(5)-La(5)#13	45.33(6)
S(6)-La(5)-La(5)#13	107.39(8)
S(10)#14-La(5)-La(5)#13	102.75(9)
S(8)#16-La(5)-La(5)#13	174.85(6)
S(8)-La(5)-La(5)#13	102.83(6)
S(4)#17-La(5)-La(5)#13	107.46(5)
S(5)#13-La(5)-La(5)#13	55.92(6)
Ti(2)-La(5)-La(5)#13	89.17(5)
S(7)#2-Ti(1)-S(7)	180.0
S(7)#2-Ti(1)-S(1)#2	89.61(9)
S(7)-Ti(1)-S(1)#2	90.39(9)
S(7)#2-Ti(1)-S(1)	90.39(9)
S(7)-Ti(1)-S(1)	89.61(9)
S(1)#2-Ti(1)-S(1)	180.0
S(7)#2-Ti(1)-S(4)#2	89.55(9)
S(7)-Ti(1)-S(4)#2	90.45(9)
S(1)#2-Ti(1)-S(4)#2	83.61(9)
S(1)-Ti(1)-S(4)#2	96.39(9)
S(7)#2-Ti(1)-S(4)	90.45(9)
S(7)-Ti(1)-S(4)	89.55(9)
S(1)#2-Ti(1)-S(4)	96.39(9)
S(1)-Ti(1)-S(4)	83.61(9)
S(4)#2-Ti(1)-S(4)	180.0
S(7)#2-Ti(1)-Ti(3)#1	90.46(7)
S(7)-Ti(1)-Ti(3)#1	89.54(7)
S(1)#2-Ti(1)-Ti(3)#1	132.32(7)
S(1)-Ti(1)-Ti(3)#1	47.68(7)
S(4)#2-Ti(1)-Ti(3)#1	48.72(7)
S(4)-Ti(1)-Ti(3)#1	131.28(7)
S(7)#2-Ti(1)-Ti(3)#6	89.54(7)
S(7)-Ti(1)-Ti(3)#6	90.46(7)
S(1)#2-Ti(1)-Ti(3)#6	47.68(7)
S(1)-Ti(1)-Ti(3)#6	132.32(7)
S(4)#2-Ti(1)-Ti(3)#6	131.28(7)
S(4)-Ti(1)-Ti(3)#6	48.72(7)
Ti(3)#1-Ti(1)-Ti(3)#6	180.0
S(3)-Ti(2)-S(8)#4	89.17(12)

S(3)-Ti(2)-S(8)	89.17(12)
S(8)#4-Ti(2)-S(8)	94.1(2)
S(3)-Ti(2)-S(5)	88.71(13)
S(8)#4-Ti(2)-S(5)	175.47(14)
S(8)-Ti(2)-S(5)	89.91(9)
S(3)-Ti(2)-S(5)#4	88.71(13)
S(8)#4-Ti(2)-S(5)#4	89.91(9)
S(8)-Ti(2)-S(5)#4	175.47(14)
S(5)-Ti(2)-S(5)#4	86.0(2)
S(3)-Ti(2)-S(6)	178.6(2)
S(8)#4-Ti(2)-S(6)	91.79(12)
S(8)-Ti(2)-S(6)	91.79(12)
S(5)-Ti(2)-S(6)	90.25(12)
S(5)#4-Ti(2)-S(6)	90.25(12)
S(3)-Ti(2)-La(2)#3	57.18(11)
S(8)#4-Ti(2)-La(2)#3	54.51(8)
S(8)-Ti(2)-La(2)#3	54.51(8)
S(5)-Ti(2)-La(2)#3	127.01(9)
S(5)#4-Ti(2)-La(2)#3	127.01(9)
S(6)-Ti(2)-La(2)#3	124.23(12)
S(3)-Ti(2)-La(4)#13	127.22(14)
S(8)#4-Ti(2)-La(4)#13	123.46(9)
S(8)-Ti(2)-La(4)#13	123.46(9)
S(5)-Ti(2)-La(4)#13	55.37(8)
S(5)#4-Ti(2)-La(4)#13	55.37(8)
S(6)-Ti(2)-La(4)#13	51.36(9)
La(2)#3-Ti(2)-La(4)#13	175.59(9)
S(3)-Ti(2)-La(1)#4	56.23(4)
S(8)#4-Ti(2)-La(1)#4	52.77(7)
S(8)-Ti(2)-La(1)#4	127.69(11)
S(5)-Ti(2)-La(1)#4	122.86(12)
S(5)#4-Ti(2)-La(1)#4	53.73(7)
S(6)-Ti(2)-La(1)#4	123.73(4)
La(2)#3-Ti(2)-La(1)#4	73.30(5)
La(4)#13-Ti(2)-La(1)#4	108.85(5)
S(3)-Ti(2)-La(1)	56.23(4)
S(8)#4-Ti(2)-La(1)	127.69(11)
S(8)-Ti(2)-La(1)	52.77(7)
S(5)-Ti(2)-La(1)	53.73(7)
S(5)#4-Ti(2)-La(1)	122.86(12)
S(6)-Ti(2)-La(1)	123.73(4)
La(2)#3-Ti(2)-La(1)	73.30(5)
La(4)#13-Ti(2)-La(1)	108.85(5)
La(1)#4-Ti(2)-La(1)	112.43(8)
S(3)-Ti(2)-La(5)	129.31(4)
S(8)#4-Ti(2)-La(5)	121.77(11)
S(8)-Ti(2)-La(5)	53.03(7)
S(5)-Ti(2)-La(5)	62.50(8)
S(5)#4-Ti(2)-La(5)	126.16(11)
S(6)-Ti(2)-La(5)	50.83(4)
La(2)#3-Ti(2)-La(5)	106.61(5)
La(4)#13-Ti(2)-La(5)	70.80(5)
La(1)#4-Ti(2)-La(5)	173.63(8)
La(1)-Ti(2)-La(5)	73.30(2)
S(3)-Ti(2)-La(5)#4	129.31(4)
S(8)#4-Ti(2)-La(5)#4	53.03(7)
S(8)-Ti(2)-La(5)#4	121.77(11)
S(5)-Ti(2)-La(5)#4	126.16(11)

S(5)#4-Ti(2)-La(5)#4	62.50(8)
S(6)-Ti(2)-La(5)#4	50.83(4)
La(2)#3-Ti(2)-La(5)#4	106.61(5)
La(4)#13-Ti(2)-La(5)#4	70.80(5)
La(1)#4-Ti(2)-La(5)#4	73.30(2)
La(1)-Ti(2)-La(5)#4	173.63(8)
La(5)-Ti(2)-La(5)#4	100.84(7)
O(2)#10-Ti(3)-O(1)	170.2(3)
O(2)#10-Ti(3)-S(1)#1	93.4(3)
O(1)-Ti(3)-S(1)#1	93.5(2)
O(2)#10-Ti(3)-S(4)#9	91.1(3)
O(1)-Ti(3)-S(4)#9	94.2(2)
S(1)#1-Ti(3)-S(4)#9	102.48(12)
O(2)#10-Ti(3)-S(2)	86.9(3)
O(1)-Ti(3)-S(2)	85.8(2)
S(1)#1-Ti(3)-S(2)	92.30(12)
S(4)#9-Ti(3)-S(2)	165.18(13)
O(2)#10-Ti(3)-S(2)#18	86.3(3)
O(1)-Ti(3)-S(2)#18	85.2(2)
S(1)#1-Ti(3)-S(2)#18	164.48(14)
S(4)#9-Ti(3)-S(2)#18	93.05(12)
S(2)-Ti(3)-S(2)#18	72.2(2)
O(2)#10-Ti(3)-Ti(3)#11	40.5(2)
O(1)-Ti(3)-Ti(3)#11	129.8(2)
S(1)#1-Ti(3)-Ti(3)#11	116.00(8)
S(4)#9-Ti(3)-Ti(3)#11	115.69(8)
S(2)-Ti(3)-Ti(3)#11	55.20(6)
S(2)#18-Ti(3)-Ti(3)#11	55.57(6)
O(2)#10-Ti(3)-Ti(3)#1	130.5(2)
O(1)-Ti(3)-Ti(3)#1	39.8(2)
S(1)#1-Ti(3)-Ti(3)#1	116.34(11)
S(4)#9-Ti(3)-Ti(3)#1	117.07(11)
S(2)-Ti(3)-Ti(3)#1	55.30(9)
S(2)#18-Ti(3)-Ti(3)#1	54.53(9)
Ti(3)#11-Ti(3)-Ti(3)#1	90.0
O(2)#10-Ti(3)-Ti(1)#1	94.2(2)
O(1)-Ti(3)-Ti(1)#1	95.5(3)
S(1)#1-Ti(3)-Ti(1)#1	51.19(8)
S(4)#9-Ti(3)-Ti(1)#1	51.29(7)
S(2)-Ti(3)-Ti(1)#1	143.49(10)
S(2)#18-Ti(3)-Ti(1)#1	144.33(11)
Ti(3)#11-Ti(3)-Ti(1)#1	134.68(3)
Ti(3)#1-Ti(3)-Ti(1)#1	135.32(3)
O(2)#10-Ti(3)-La(1)	147.2(3)
O(1)-Ti(3)-La(1)	37.97(13)
S(1)#1-Ti(3)-La(1)	55.84(8)
S(4)#9-Ti(3)-La(1)	105.49(9)
S(2)-Ti(3)-La(1)	83.56(7)
S(2)#18-Ti(3)-La(1)	119.93(9)
Ti(3)#11-Ti(3)-La(1)	138.56(3)
Ti(3)#1-Ti(3)-La(1)	66.31(4)
Ti(1)#1-Ti(3)-La(1)	75.91(4)
O(2)#10-Ti(3)-La(1)#1	145.3(3)
O(1)-Ti(3)-La(1)#1	37.78(13)
S(1)#1-Ti(3)-La(1)#1	105.20(10)
S(4)#9-Ti(3)-La(1)#1	56.75(7)
S(2)-Ti(3)-La(1)#1	120.47(9)
S(2)#18-Ti(3)-La(1)#1	83.11(7)

Ti(3)#11-Ti(3)-La(1)#1	138.45(3)
Ti(3)#1-Ti(3)-La(1)#1	66.08(4)
Ti(1)#1-Ti(3)-La(1)#1	76.35(4)
La(1)-Ti(3)-La(1)#1	63.40(4)
O(2)#10-Ti(3)-La(3)#10	37.9(3)
O(1)-Ti(3)-La(3)#10	147.40(12)
S(1)#1-Ti(3)-La(3)#10	55.86(8)
S(4)#9-Ti(3)-La(3)#10	102.57(8)
S(2)-Ti(3)-La(3)#10	84.80(9)
S(2)#18-Ti(3)-La(3)#10	121.09(8)
Ti(3)#11-Ti(3)-La(3)#10	66.60(3)
Ti(3)#1-Ti(3)-La(3)#10	139.95(8)
Ti(1)#1-Ti(3)-La(3)#10	74.52(4)
La(1)-Ti(3)-La(3)#10	109.82(5)
La(1)#1-Ti(3)-La(3)#10	150.85(6)
Ti(3)#1-S(1)-Ti(1)	81.13(10)
Ti(3)#1-S(1)-La(1)#1	85.49(9)
Ti(1)-S(1)-La(1)#1	98.83(9)
Ti(3)#1-S(1)-La(3)#2	85.69(10)
Ti(1)-S(1)-La(3)#2	96.78(8)
La(1)#1-S(1)-La(3)#2	160.65(10)
Ti(3)-S(2)-Ti(3)#11	69.60(12)
Ti(3)-S(2)-Ti(3)#18	107.8(2)
Ti(3)#11-S(2)-Ti(3)#18	70.17(10)
Ti(3)-S(2)-Ti(3)#1	70.17(10)
Ti(3)#11-S(2)-Ti(3)#1	107.82(14)
Ti(3)#18-S(2)-Ti(3)#1	68.85(12)
Ti(2)-S(3)-La(2)#3	84.86(13)
Ti(2)-S(3)-La(1)	86.39(7)
La(2)#3-S(3)-La(1)	90.80(7)
Ti(2)-S(3)-La(1)#4	86.39(7)
La(2)#3-S(3)-La(1)#4	90.80(7)
La(1)-S(3)-La(1)#4	172.43(14)
Ti(2)-S(3)-La(3)	88.02(13)
La(2)#3-S(3)-La(3)	172.88(14)
La(1)-S(3)-La(3)	88.74(7)
La(1)#4-S(3)-La(3)	88.74(7)
Ti(3)#6-S(4)-Ti(1)	79.99(9)
Ti(3)#6-S(4)-La(2)	86.62(10)
Ti(1)-S(4)-La(2)	99.82(8)
Ti(3)#6-S(4)-La(5)#5	152.75(12)
Ti(1)-S(4)-La(5)#5	127.26(10)
La(2)-S(4)-La(5)#5	88.31(7)
Ti(3)#6-S(4)-La(1)#2	83.87(8)
Ti(1)-S(4)-La(1)#2	98.15(9)
La(2)-S(4)-La(1)#2	157.86(10)
La(5)#5-S(4)-La(1)#2	91.05(7)
Ti(2)-S(5)-La(3)	87.28(10)
Ti(2)-S(5)-La(1)	84.37(9)
La(3)-S(5)-La(1)	93.09(8)
Ti(2)-S(5)-La(4)#13	82.64(10)
La(3)-S(5)-La(4)#13	92.60(8)
La(1)-S(5)-La(4)#13	165.55(11)
Ti(2)-S(5)-La(5)#13	152.27(13)
La(3)-S(5)-La(5)#13	120.41(10)
La(1)-S(5)-La(5)#13	92.07(8)
La(4)#13-S(5)-La(5)#13	96.48(8)
Ti(2)-S(6)-La(4)#13	84.85(12)

Ti(2)-S(6)-La(5)	86.85(8)
La(4)#13-S(6)-La(5)	95.90(7)
Ti(2)-S(6)-La(5)#4	86.85(8)
La(4)#13-S(6)-La(5)#4	95.90(7)
La(5)-S(6)-La(5)#4	166.1(2)
Ti(2)-S(6)-La(2)#17	148.4(2)
La(4)#13-S(6)-La(2)#17	126.75(14)
La(5)-S(6)-La(2)#17	89.43(8)
La(5)#4-S(6)-La(2)#17	89.43(8)
Ti(1)-S(7)-La(3)	101.96(8)
Ti(1)-S(7)-La(1)#1	101.85(9)
La(3)-S(7)-La(1)#1	156.19(10)
Ti(1)-S(7)-La(1)	101.78(9)
La(3)-S(7)-La(1)	94.13(8)
La(1)#1-S(7)-La(1)	81.18(6)
Ti(1)-S(7)-La(2)	100.80(8)
La(3)-S(7)-La(2)	81.93(7)
La(1)#1-S(7)-La(2)	93.45(8)
La(1)-S(7)-La(2)	157.41(10)
Ti(2)-S(8)-La(1)	85.54(9)
Ti(2)-S(8)-La(2)#3	83.22(10)
La(1)-S(8)-La(2)#3	95.06(8)
Ti(2)-S(8)-La(5)#16	150.00(13)
La(1)-S(8)-La(5)#16	124.37(10)
La(2)#3-S(8)-La(5)#16	90.98(7)
Ti(2)-S(8)-La(5)	86.46(10)
La(1)-S(8)-La(5)	96.60(8)
La(2)#3-S(8)-La(5)	163.77(11)
La(5)#16-S(8)-La(5)	91.73(8)
La(4)-S(9)-La(1)	138.91(12)
La(4)-S(9)-La(5)	110.21(11)
La(1)-S(9)-La(5)	103.94(11)
La(4)-S(9)-La(5)#13	100.06(10)
La(1)-S(9)-La(5)#13	102.55(11)
La(5)-S(9)-La(5)#13	89.33(9)
S(11)#19-S(10)-S(11)#11	78.4(3)
S(11)#19-S(10)-La(5)#12	142.25(12)
S(11)#11-S(10)-La(5)#12	105.57(12)
S(11)#19-S(10)-La(5)#20	105.57(12)
S(11)#11-S(10)-La(5)#20	142.25(12)
La(5)#12-S(10)-La(5)#20	93.8(2)
S(11)#19-S(10)-La(4)#20	56.8(2)
S(11)#11-S(10)-La(4)#20	55.1(2)
La(5)#12-S(10)-La(4)#20	154.37(4)
La(5)#20-S(10)-La(4)#20	94.88(3)
S(11)#19-S(10)-La(4)#15	55.1(2)
S(11)#11-S(10)-La(4)#15	56.8(2)
La(5)#12-S(10)-La(4)#15	94.88(3)
La(5)#20-S(10)-La(4)#15	154.37(4)
La(4)#20-S(10)-La(4)#15	87.5(2)
S(11)#4-S(11)-S(10)#19	140.8(2)
S(11)#4-S(11)-La(4)#7	80.25(12)
S(10)#19-S(11)-La(4)#7	77.9(2)
S(11)#4-S(11)-La(3)	80.34(12)
S(10)#19-S(11)-La(3)	134.9(2)
La(4)#7-S(11)-La(3)	140.7(2)
S(11)#4-S(11)-La(4)#13	80.50(12)
S(10)#19-S(11)-La(4)#13	76.5(2)

La(4)#7-S(11)-La(4)#13	109.0(2)
La(3)-S(11)-La(4)#13	101.1(2)
Ti(3)#1-O(1)-Ti(3)	100.5(5)
Ti(3)#1-O(1)-La(1)#1	113.13(6)
Ti(3)-O(1)-La(1)#1	113.44(6)
Ti(3)#1-O(1)-La(1)	113.44(6)
Ti(3)-O(1)-La(1)	113.13(6)
La(1)#1-O(1)-La(1)	103.7(4)
Ti(3)#6-O(2)-Ti(3)#7	99.0(4)
Ti(3)#6-O(2)-La(2)	114.3(3)
Ti(3)#7-O(2)-La(2)	114.3(3)
Ti(3)#6-O(2)-La(3)	113.5(3)
Ti(3)#7-O(2)-La(3)	113.5(3)
La(2)-O(2)-La(3)	102.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+2	#2 -x+1/2,-y+3/2,-z+2
#3 -x+1,-y+2,-z+2	#4 x,-y+2,z
#5 x,y,z+1	#6 x-1/2,-y+3/2,z
#7 x-1/2,y+1/2,z	#8 -x+1/2,y+1/2,-z+2
#9 x+1/2,-y+3/2,z	#10 x+1/2,y-1/2,z
#11 x,-y+1,z	#12 -x+1/2,y-1/2,-z+1
#13 -x+1/2,-y+3/2,-z+1	#14 x+1/2,y+1/2,z
#15 -x+1/2,-y+1/2,-z+1	#16 -x+1,y,-z+1
#17 x,y,z-1	#18 -x+1,-y+1,-z+2
#19 -x,-y+1,-z+1	#20 x-1/2,y-1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for UM178. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
La(1)	5(1)	10(1)	13(1)	1(1)	5(1)	0(1)
La(2)	5(1)	8(1)	13(1)	0	4(1)	0
La(3)	5(1)	10(1)	11(1)	0	4(1)	0
La(4)	7(1)	31(1)	18(1)	0	7(1)	0
La(5)	19(1)	23(1)	24(1)	6(1)	3(1)	-8(1)
Ti(1)	6(1)	11(2)	16(2)	-1(1)	8(1)	-1(1)
Ti(2)	9(1)	13(2)	18(2)	0	5(1)	0
Ti(3)	4(1)	7(1)	14(1)	1(1)	5(1)	1(1)
S(1)	6(1)	11(1)	16(1)	-2(1)	6(1)	-1(1)
S(2)	6(2)	9(2)	13(2)	0	6(2)	0
S(3)	8(2)	8(2)	13(2)	0	6(2)	0
S(4)	6(1)	9(1)	14(1)	0(1)	6(1)	-1(1)
S(5)	10(1)	13(2)	18(2)	1(1)	0(1)	-2(1)
S(6)	10(2)	12(2)	16(2)	0	9(2)	0
S(7)	5(1)	8(1)	16(1)	-1(1)	7(1)	-1(1)
S(8)	7(1)	9(1)	16(1)	-1(1)	6(1)	0(1)
S(9)	32(2)	14(2)	15(2)	1(1)	-1(1)	-10(1)
S(10)	9(3)	11(4)	16(4)	0	4(3)	0
S(11)	6(2)	20(3)	15(3)	9(2)	4(2)	1(2)
O(1)	3(5)	7(5)	14(5)	0	4(4)	0
O(2)	1(5)	9(6)	12(5)	0	2(4)	0

Rietveld .rie file for $La_{14}Ti_8S_{33}O_4$ (UM178)

```
   1   1   0   0   0   0   0   0
   1   0   1   1   1   1   1   1   0   1   0   0
   1
   6
 0.00000 0.00000  0.0000 15.0000  0.0000 10.0000  0.0300 59.9800
  0.3000  1.0000  1.0000  1.0000  1.0000
   0     0.14538 0.00000
           0.00    0.00
-2.80795e+03-2.52099e+02-7.61131e+00-9.94775e-02-4.78295e-04 0.00000e+00
    0.00         0.00         0.00         0.00         0.00         0.00
   1   1   1   1   1   1   1
UM178
C 2/m                   3                  4.56454
  21   0   0   0   0   2   0   0   0   0
O2      O-2     0         0.16822 1.00000-0.02251 0.05000 1.00000
                             0.00    0.00    0.00    0.00    0.00
                          0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                             0.00    0.00    0.00    0.00    0.00    0.00
O1      O-2     0         0.50000 0.67878 1.00000 1.79190 1.00000
                             0.00    0.00    0.00    0.00    0.00
                          0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                             0.00    0.00    0.00    0.00    0.00    0.00
S11     S-2     0         0.08883 0.98845 0.65218 0.05000 0.50000
                             0.00    0.00    0.00    0.00    0.00
                          0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
                             0.00    0.00    0.00    0.00    0.00    0.00
S10     S-2     0         0.00000 0.17557 0.50000 0.05000 1.00000
                             0.00    0.00    0.00    0.00    0.00
```