

Supplementary Table 1: Atomic parameters for Sr-ETS-4 in space group *Cmmm*. Values for four heat-treatment temperatures (423 K, 473 K, 523 K, and 573 K) are shown for each atom. The lattice parameters are as in Table 1. Weighted residuals (R_{wp}) are 3.40%, 4.40%, 4.51% and 4.63% respectively. The corresponding structureless (Le Bail²²) residuals (representing the best possible fits in *Cmmm*) are 1.68%, 3.09%, 3.41% and 3.56%. Also see note on estimated standard deviations (e.s.d.'s) at the foot of the Table.

Name	x	y	z	Occupancy	Multiplicity	Uiso*10 ²
Ti1	.25	.25	0	1	4	3.63(13)
	.25	.25	0	1	4	2.62(10)
	.25	.25	0	1	4	1.62(11)
	.25	.25	0	1	4	1.92(9)
Ti2	0	.5	.0409(6)	.2061(5)	4	3.63(13)
	0	.5	.0201(9)	.2154(5)	4	2.62(10)
	0	.5	.0155(10)	.2182(5)	4	1.62(11)
	0	.5	.0003(6)	.2145(5)	4	1.92(9)
Si1	.1599(4)	0	.2721(18)	1	8	3.55(5)
	.1608(5)	0	.2681(15)	1	8	3.92(6)
	.1597(7)	0	.2589(14)	1	8	2.28(4)
	.1544(6)	0	.2606(10)	1	8	4.83(4)
Si2	.0645(4)	.0818(20)	0	.4133(10)	8	3.55(5)
	.0639(5)	.0913(24)	0	.4319(9)	8	3.92(6)
	.0634(5)	.0962(29)	0	.4365(10)	8	2.28(4)
	.0655(4)	.0802(26)	0	.4290(10)	8	4.83(4)
Na1	.25	.25	.5	.1970(33)	4	13.12(34)
	.25	.25	.5	.1969(23)	4	12.86(29)
	.25	.25	.5	.1970(29)	4	14.24(28)
	.25	.25	.5	.1969(31)	4	11.23(28)
Sr1	.1374(34)	.5	.2321(8)	.2614(12)	8	1.42(4)
	.1365(29)	.5	.2127(8)	.2314(11)	8	1.94(7)
	.1371(31)	.5	.2038(9)	.2236(12)	8	2.00(7)
	.1396(32)	.5	.2025(9)	.2444(12)	8	2.07(8)
Sr2	.2086(11)	.5	.5	.5621(11)	4	1.42(4)
	.2250(11)	.5	.5	.5121(14)	4	1.94(7)
	.2349(14)	.5	.5	.5167(12)	4	2.00(7)
	.2299(14)	.5	.5	.5125(11)	4	2.07(8)
Sr3	0	0	.5	.1902(10)	2	1.42(4)
	0	0	.5	.3452(19)	2	1.94(7)
	0	0	.5	.3475(11)	2	2.00(7)
	0	0	.5	.3469(14)	2	2.07(8)
O1	.1459(19)	0	.5	1	4	9.10(35)
	.1475(10)	0	.5	1	4	14.93(11)
	.1577(12)	0	.5	1	4	25.16(19)
	.1586(15)	0	.5	1	4	43.38(37)
O2	.0953(25)	0	.1953(15)	1	8	7.30(47)
	.0962(6)	0	.1874(21)	1	8	10.12(27)
	.0939(12)	0	.1901(23)	1	8	10.38(8)
	.0865(7)	0	.2144(16)	1	8	17.76(14)

O3	.1947(34)	.1828(9)	.2071(10)	1	16	8.17(34)
	.1941(4)	.1910(11)	.2183(12)	1	16	11.47(35)
	.1908(4)	.1997(14)	.2131(13)	1	16	14.23(36)
	.1878(6)	.2027(15)	.2051(20)	1	16	28.95(15)
O4	.2180(8)	.5	0	1	4	7.86(66)
	.2123(7)	.5	0	1	4	14.72(62)
	.2059(6)	.5	0	1	4	20.90(23)
	.2032(7)	.5	0	1	4	80.04(71)
O5	0	0	0	.8265(20)	2	6.86(70)
	0	0	0	.8638(18)	2	9.28(15)
	0	0	0	.8730(20)	2	7.23(16)
	0	0	0	.8580(20)	2	21.66(33)
O6	.0632(49)	.3095(21)	0	.4133(10)	8	12.71(113)
	.0680(27)	.3218(24)	0	.4319(9)	8	26.29(135)
	.0707(7)	.3292(27)	0	.4365(10)	8	18.92(129)
	.0702(6)	.3206(25)	0	.4290(10)	8	15.13(126)
O7	0	.5	.2970(65)	.2061(5)	4	15.80(312)
	0	.5	.2761(92)	.2154(5)	4	21.46(148)
	0	.5	.2404(98)	.2182(5)	4	23.68(179)
	0	.5	.2576(62)	.2145(5)	4	11.31(153)
O _w	.1174(21)	.5	.5	.3713(39)	4	10.70(45)
	.1168(19)	.5	.5	.1928(18)	4	17.43(63)
	.1221(23)	.5	.5	.1005(16)	4	12.95(51)
	.1262(21)	.5	.5	.0550(23)	4	13.38(49)

Note: All e.s.d.'s are given as errors on the last reported decimal digit. For example, a value of 0.1262(21) for the *x* fractional coordinate of O_w (last row in Table) means 0.1262±0.0021, and the isotropic atomic displacement parameter, U_{iso} is (13.38±0.49)/100 = 0.1338±0.0049 Å².