Titanite, $CaTiSiO_5$

This mineral displays more than one symmetry. Analyses are given for each.

Titanite
Ghose S, Ito Y, Hatch D M
Physics and Chemistry of Minerals 17 (1991) 591-603
Paraelectric-antiferroelectric phase transition in titanite, CaTiSiO5
I. A high temperature X-ray diffraction study of the order parameter and transition mechanism
7.0722 8.7302 6.5672 90 113.840 90 P2_1/a

atom	x	y	z	Wyckoff
Ca	0.2421	0.4185	0.2511	4e
Ti	0.5137	0.2540	0.7496	4e
Si	0.7483	0.4327	0.2491	4e
O1	0.7494	0.3219	0.7491	4e
O2	0.9097	0.3161	0.4332	4e
O3	0.0881	0.1849	0.0644	4e
O4	0.3829	0.4609	0.6456	4e
O5	0.6191	0.0399	0.8532	4e

(8 × 4e)

Raman Active Modes

WP	A_g	A_u	B_g	B_u
4e	3	·	3	·

Total number of modes:
$24A_g + 24B_g = 48$

Titanite, $CaTiSiO_5$

Titanite
Hawthorne F C, Groat L A, Raudsepp M, Ball N A, Kimata M, Spike F D, Gaba R, Halden N M, Lumpkin G R, Ewing R C, Greegor R B, Lytle F W, Ercit T S, Rossman G R, Wicks F J, Ramik R A, Sherriff B L, Fleet M E, McCammon C A
American Mineralogist 76 (1991) 370-396
Alpha-decay damage in titanite
6.549 8.695 7.060 90 113.87 90 C2/c

atom	x	y	z	Wyckoff
Ca	0	0.1677	0.75	4e
Ti	0	0.5	0	4b
Si	0	0.1828	0.25	4e
O1	0	0.5714	0.25	4e
O2	0.1855	0.0663	0.4102	8f
O3	0.1025	0.2893	0.1185	8f

$(2 \times 8f) + (3 \times 4e) + (1 \times 4b)$

Raman Active Modes

WP	A_g	A_u	B_g	B_u
8f	3	·	3	·
4e	1	·	2	·
4b	·	·	·	·

Total number of modes:
$9A_g + 12B_g = 21$