

$\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Ca}_{0.5}\text{Tm}_{11}\text{O}_{18}$ $hP72$ $(176) P6_3/m - h^{10} \text{fdcba}$ **BaSrCaTm₂₂O₃₆** [1]

Structural features: Double infinite chains of edge-linked TmO_6 octahedra and single columns of base-linked $(\text{Tm,Ca})\text{O}_6$ trigonal prisms (partial vacancies ignored) share atoms to form a 3D-framework; (Ba,Sr) and additional Ca in channels parallel to [001] (partial disorder). Variant of $\text{Ba}_2\text{SrLu}_{22}\text{O}_{36}$.

Krüger J., Müller Buschbaum H. (1982) [1]

 $\text{Ba}_{0.50}\text{Ca}_{0.50}\text{O}_{18}\text{Sr}_{0.50}\text{Tm}_{11}$ $a = 1.76, c = 0.3353 \text{ nm}, c/a = 0.191, V = 0.8995 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6h	m..	0.023	0.164	$\frac{1}{4}$		non-coplanar triangle Tm_3
O2	6h	m..	0.028	0.58	$\frac{1}{4}$		square pyramid Tm_5
O3	6h	m..	0.172	0.538	$\frac{1}{4}$		non-coplanar triangle Tm_3
Tm4	6h	m..	0.212	0.434	$\frac{1}{4}$		octahedron O_6
O5	6h	m..	0.215	0.307	$\frac{1}{4}$		square pyramid Tm_5
Tm6	6h	m..	0.2309	0.1202	$\frac{1}{4}$		octahedron O_6
M7	6h	m..	0.3378	0.0093	$\frac{1}{4}$	0.75	trigonal prism O_6
O8	6h	m..	0.357	0.249	$\frac{1}{4}$		square pyramid Tm_5
O9	6h	m..	0.486	0.185	$\frac{1}{4}$		non-coplanar triangle Tm_3
Tm10	6h	m..	0.5509	0.103	$\frac{1}{4}$		octahedron O_6
M11	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0	0.209	
M12	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.208	
M13	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.208	
M14	2b	-3..	0	0	0	0.167	
Ca15	2a	-6..	0	0	$\frac{1}{4}$	0.25	

$\text{M7} = 0.889\text{Tm} + 0.111\text{Ca}$; $\text{M11} = 0.5\text{Ba} + 0.5\text{Sr}$; $\text{M12} = 0.5\text{Ba} + 0.5\text{Sr}$; $\text{M13} = 0.5\text{Ba} + 0.5\text{Sr}$; $\text{M14} = 0.5\text{Ba} + 0.5\text{Sr}$

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.090$

Remarks: Metastable phase. Short interatomic distances for partly occupied site(s).

References: [1] Krüger J., Müller Buschbaum H. (1982), Z. Anorg. Allg. Chem. 494, 103-108.