

$\text{K}_{0.5}\text{CaYb}_{1.83}\text{S}_4$  $hP18$  $(186) P6_3mc - b^6a^3$  **$\text{K}_{0.5}\text{CaYb}_{1.83}\text{S}_4$  [1]**

Structural features: Close-packed S layers in ABCAACBA stacking; Ca and Yb in octahedral, K in trigonal prismatic voids (partial disorder for the latter). Ignoring vacancies, triple slabs of edge-linked  $\text{YbS}_6$  and  $\text{CaS}_6$  octahedra.

El Fadli Z. et al. (1994) [1]

 $\text{CaK}_{0.50}\text{S}_4\text{Yb}_{1.83}$  $a = 0.3901$ ,  $c = 2.935$  nm,  $c/a = 7.524$ ,  $V = 0.3868$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	$2b$	$3m.$	$1/3$	$2/3$	0.0986		octahedron $\text{Yb}_3\text{Ca}_3$
Yb2	$2b$	$3m.$	$1/3$	$2/3$	0.2711		octahedron $\text{S}_6$
K3	$2b$	$3m.$	$1/3$	$2/3$	0.4105	0.25	coplanar triangle $\text{K}_3$
Yb4	$2b$	$3m.$	$1/3$	$2/3$	0.5453	0.833	octahedron $\text{S}_6$
S5	$2b$	$3m.$	$1/3$	$2/3$	0.7155		octahedron $\text{Yb}_3\text{Ca}_3$
K6	$2b$	$3m.$	$1/3$	$2/3$	0.9105	0.25	coplanar triangle $\text{K}_3$
S7	$2a$	$3m.$	0	0	0.0		non-coplanar triangle $\text{Yb}_3$
Ca8	$2a$	$3m.$	0	0	0.1533		octahedron $\text{S}_6$
S9	$2a$	$3m.$	0	0	0.3218		non-coplanar triangle $\text{Yb}_3$

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.5215Experimental: single crystal, diffractometer, X-rays,  $R = 0.043$ ,  $T = 293$  K

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

References: [1] El Fadli Z., Lemoine P., Tomas A. (1994), Acta Crystallogr. C 50, 1373-1375.