

$\text{Cs}_{0.35}\text{V}_3\text{O}_7$ $hP24$ $(176) P6_3/m - h^3cba$ $\text{Cs}_{0.35}\text{V}_3\text{O}_7$ [1]

Structural features: Double infinite chains of edge-linked VO_5 square pyramids share vertices to form a 3D-framework; Cs in channels parallel to $[001]$ (partial disorder).

Waltersson K., Forslund B. (1977) [1]

 $\text{Cs}_{0.35}\text{O}_7\text{V}_3$ $a = 0.988$, $c = 0.3605$ nm, $c/a = 0.365$, $V = 0.3048$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
V1	$6h$	$m..$	0.12185	0.50329	$1/4$		square pyramid O_5
O2	$6h$	$m..$	0.1349	0.3511	$1/4$		single atom V
O3	$6h$	$m..$	0.5484	0.0963	$1/4$		non-coplanar triangle V_3
O4	$2c$	$-6..$	$1/3$	$2/3$	$1/4$		coplanar triangle V_3
Cs5	$2b$	$-3..$	0	0	0	0.186	
Cs6	$2a$	$-6..$	0	0	$1/4$	0.162	

Transformation from published data: $y, x, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.032$

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

References: [1] Waltersson K., Forslund B. (1977), Acta Crystallogr. B 33, 775-779.