

Cs<sub>0.3</sub>V<sub>2</sub>O<sub>5</sub>

hP48

(176)  $P6_3/m - h^7ed$ **Cs<sub>0.3</sub>V<sub>2</sub>O<sub>5</sub>** [1]

Structural features: Double infinite chains of edge-linked VO<sub>5</sub> square pyramids share vertices to form tubes (12 pyramids in the cross-section); Cs in and between the tubes (partial disorder).

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

Cs<sub>0.31</sub>O<sub>5</sub>V<sub>2</sub> $a = 1.436$ ,  $c = 0.3611$  nm,  $c/a = 0.251$ ,  $V = 0.6449$  nm<sup>3</sup>,  $Z = 6$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
V1	6 <i>h</i>	<i>m</i> ..	0.08696	0.42593	$\frac{1}{4}$		square pyramid O <sub>5</sub>
O2	6 <i>h</i>	<i>m</i> ..	0.09859	0.54223	$\frac{1}{4}$		single atom V
O3	6 <i>h</i>	<i>m</i> ..	0.15147	0.24499	$\frac{1}{4}$		single atom V
O4	6 <i>h</i>	<i>m</i> ..	0.22403	0.45382	$\frac{1}{4}$		non-colinear V <sub>2</sub>
V5	6 <i>h</i>	<i>m</i> ..	0.26261	0.35248	$\frac{1}{4}$		square pyramid O <sub>5</sub>
O6	6 <i>h</i>	<i>m</i> ..	0.37254	0.06385	$\frac{1}{4}$		non-coplanar triangle V <sub>3</sub>
O7	6 <i>h</i>	<i>m</i> ..	0.38002	0.31732	$\frac{1}{4}$		non-coplanar triangle V <sub>3</sub>
Cs8	4 <i>e</i>	3..	0	0	0.13175	0.162	
Cs9	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.618	trigonal prism O <sub>6</sub>

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0  $\frac{1}{2}$ 

Experimental: single crystal, diffractometer, X-rays, wR = 0.038

Remarks: Average structure; additional reflections could be indexed with a 7-fold supercell (new axes a,b,7c). Short interatomic distances for partly occupied site(s).

References: [1] Waltersson K., Forslund B. (1977), Acta Crystallogr. B 33, 780-784.