

$V_{12}P_7$	$hP26$	$(176) P6_3/m - h^4a$
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$V_{12}P_7$  [1];  $Cr_{12}P_7$  [2]

Structural features: Infinite columns of base-linked  $PV_6V_2$  bicapped trigonal prisms ( $PV_8$  square antiprisms; one split V site) share atoms to form a 3D-framework with WC-type columns (3 P-centered prisms in the triangular cross-section); additional P (partial disorder) in channels of hexagonal cross-section parallel to [001]. Variant of  $Th_7S_{12}$  antitype.

Olofsson O., Ganglberger E. (1970) [1]

$P_7V_{12}$

$a = 0.9299$ ,  $c = 0.3279$  nm,  $c/a = 0.353$ ,  $V = 0.2456$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
V1	$6h$	$m..$	0.1324	0.5095	$1/4$		monocapped trigonal prism $P_5V_2$
V2	$6h$	$m..$	0.1991	0.2046	$1/4$	0.5	
V3	$6h$	$m..$	0.2503	0.2646	$1/4$	0.5	
P4	$6h$	$m..$	0.4507	0.164	$1/4$		trigonal bipyramid $P_2V_3$
P5	$2a$	$-6..$	0	0	$1/4$	0.5	

Transformation from published data:  $y, x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.070$

Remarks: Short interatomic distances for partly occupied site(s). Space group (174)  $P-6$  was tested and rejected ( $R = 0.15$ ). A similar structure proposal for  $Cr_{12}P_7$  in space group (174)  $P-6$  in [3] is superseded (see [2]). Additional reflections observed for  $Cr_{12}P_7$  in [2] could be indexed with a 7-fold supercell (new axes  $2a-b, a+3b, c$ ).

References: [1] Olofsson O., Ganglberger E. (1970), Acta Chem. Scand. 24, 2389-2396. [2] Chun H.K., Carpenter G.B. (1979), Acta Crystallogr. B 35, 30-33. [3] Baurecht H.E., Boller H., Nowotny H. (1971), Monatsh. Chem. 102, 373-384.