

$\text{Cr}_{12}\text{P}_7$	$hP19$	$(174) P-6 - k^3j^3a$
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$\text{Cr}_{12}\text{P}_7$  [1];  $\text{U}_7\text{Te}_{12}$  [2];  $(\text{Mo},\text{Mn})_{12}\text{P}_7$  [3]

Structural features: Infinite columns of base-linked  $\text{PCr}_6\text{Cr}_2$  bicapped trigonal prisms ( $\text{PCr}_8$  square antiprisms) and  $\text{PCr}_6\text{Cr}_3$  tricapped trigonal prisms share atoms to form a 3D-framework with WC-type columns (3 P-centered prisms in the triangular cross-section). Derivative of  $\text{Th}_7\text{S}_{12}$  antitype with an ordered atom arrangement along the c-axis. See Fig. IV.88.

Baurecht H.E. et al. (1971) [1]

$\text{Cr}_{12}\text{P}_7$

$a = 0.8977$ ,  $c = 0.3316$  nm,  $c/a = 0.369$ ,  $V = 0.2314$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
P1	$3k$	$m..$	0.1634	0.4408	$\frac{1}{2}$		square antiprism $\text{Cr}_8$
Cr2	$3k$	$m..$	0.2231	0.2106	$\frac{1}{2}$		pseudo Frank-Kasper $\text{P}_6\text{Cr}_{12}$
Cr3	$3k$	$m..$	0.5091	0.1315	$\frac{1}{2}$		15-vertex Frank-Kasper $\text{P}_5\text{Cr}_{10}$
Cr4	$3j$	$m..$	0.0162	0.2577	0		cuboctahedron $\text{P}_4\text{Cr}_8$
Cr5	$3j$	$m..$	0.3694	0.5092	0		15-vertex Frank-Kasper $\text{P}_5\text{Cr}_{10}$
P6	$3j$	$m..$	0.4497	0.2881	0		square antiprism $\text{Cr}_8$
P7	$1a$	$-6..$	0	0	0		tricapped trigonal prism $\text{Cr}_9$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.090$

Remarks: Space group  $(176) P6_3/m$  was tested and rejected ( $R = 0.22$ ). A partly ordered arrangement of Mo and Mn was found for  $(\text{Mo},\text{Mn})_{12}\text{P}_7$  in [3],  $\text{Mo}_3(\text{Mo}_{0.6}\text{Mn}_{0.4})_6\text{Mn}_3\text{P}_7$ .

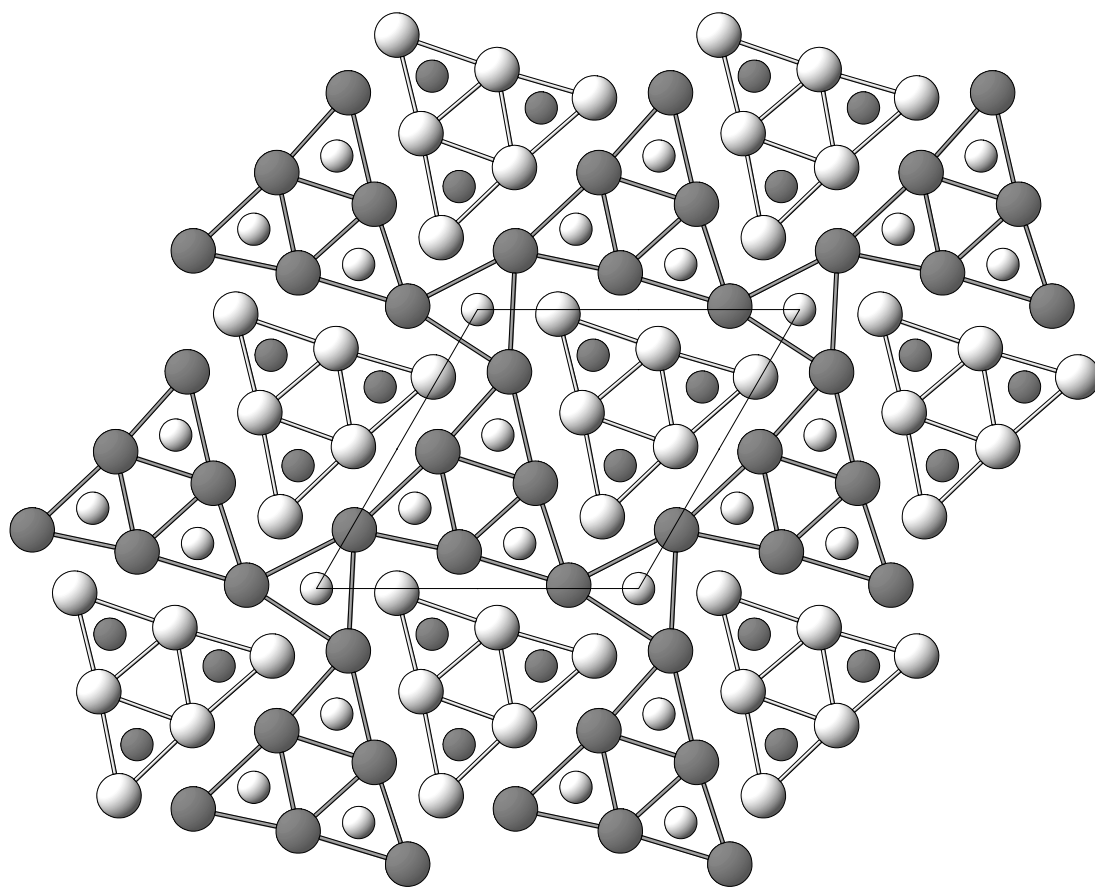


Fig. IV.88.  $\text{Cr}_{12}\text{P}_7$

Arrangement of  $\text{PCr}_6$  trigonal prisms (P atoms small, Cr atoms large) viewed along  $[001]$ .  
Light and dark atoms are shifted by  $c/2$ .

References: [1] Baurecht H.E., Boller H., Nowotny H. (1971), *Monatsh. Chem.* 102, 373-384. [2] Tougait O., Potel M., Noel H. (1998), *Inorg. Chem.* 37, 5088-5091. [3] Oryshchin S.V., Zhak O.V., Députier S., Le Sénéchal C., Guérin R. (2004), *Inorg. Mater.* 40, 616-622 (*Neorg. Mater.* 40, 709-715).