

$\text{Zr}_3\text{Cr}_{30}\text{P}_{19.5}$ $hP112$ $(176) P6_3/m - h^{18}\text{da}$ **Zr₆Cr₆₀P₃₉** [1]

Structural features: Infinite columns of base-linked $\text{P}(\text{Zr}_2\text{Cr}_4)\text{Cr}_2$ and PCr_6Cr_2 bicapped and PCr_6Cr_3 tricapped trigonal prisms share atoms to form a 3D-framework with triple "extended" propeller-like columns (nine additional outer prism columns) centered by a prism column shifted by $c/2$.

Le Sénéchal C. et al. (1999) [1]

 $\text{Cr}_{30}\text{P}_{19.50}\text{Zr}_3$ $a = 2.1413$, $c = 0.3354$ nm, $c/a = 0.157$, $V = 1.3318$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	6h	m..	0.0346	0.5941	$\frac{1}{4}$		square antiprism Cr ₈
P2	6h	m..	0.0395	0.1792	$\frac{1}{4}$		
Cr3	6h	m..	0.0462	0.4258	$\frac{1}{4}$		tetrahedron P ₄
P4	6h	m..	0.0898	0.3454	$\frac{1}{4}$		square antiprism Cr ₆ Zr ₂
Cr5	6h	m..	0.0995	0.0503	$\frac{1}{4}$	0.5	
Cr6	6h	m..	0.124	0.0623	$\frac{1}{4}$	0.5	
P7	6h	m..	0.1467	0.5423	$\frac{1}{4}$		square antiprism Cr ₆ Zr ₂
Cr8	6h	m..	0.1643	0.2105	$\frac{1}{4}$		square pyramid P ₅
Cr9	6h	m..	0.2053	0.3605	$\frac{1}{4}$		tetrahedron P ₄
Cr10	6h	m..	0.269	0.1707	$\frac{1}{4}$		square pyramid P ₅
Cr11	6h	m..	0.2699	0.5836	$\frac{1}{4}$		tetrahedron P ₄
P12	6h	m..	0.2867	0.4844	$\frac{1}{4}$		square antiprism Cr ₆ Zr ₂
P13	6h	m..	0.2992	0.0745	$\frac{1}{4}$		square antiprism Cr ₈
Cr14	6h	m..	0.3097	0.3131	$\frac{1}{4}$		square pyramid P ₅
Cr15	6h	m..	0.4252	0.1041	$\frac{1}{4}$		square pyramid P ₅
Zr16	6h	m..	0.4572	0.2829	$\frac{1}{4}$		trigonal prism P ₆
Cr17	6h	m..	0.5286	0.0621	$\frac{1}{4}$		square pyramid P ₅
Cr18	6h	m..	0.5696	0.2049	$\frac{1}{4}$		square pyramid P ₅
P19	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cr ₉
P20	2a	-6..	0	0	$\frac{1}{4}$	0.5	trigonal bipyramid P ₂ Cr ₃

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.053$, $T = 293$ K

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

References: [1] Le Sénéchal C., Babizhetskii V., Députier S., Pivan J.Y., Guérin R. (1999), J. Solid State Chem. 144, 277-286.