

$\text{Zr}_2\text{Cr}_{30}\text{P}_{19}$ $hP51$ (174) $P-6 - k^8j^8eda$ **Zr₂Cr₃₀P₁₉** [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 extended propeller-like columns (two additional columns attached to each blade).

Le Sénéchal C. et al. (1998) [1]

 $\text{Cr}_{30}\text{P}_{19}\text{Zr}_2$ $a = 1.4807$, $c = 0.3348$ nm, $c/a = 0.226$, $V = 0.6357$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	$3k$	$m..$	0.048	0.4094	$\frac{1}{2}$		square antiprism Cr ₈
Cr2	$3k$	$m..$	0.0571	0.1454	$\frac{1}{2}$		pseudo Frank-Kasper P ₆ Cr ₁₂
Cr3	$3k$	$m..$	0.0665	0.5853	$\frac{1}{2}$		cuboctahedron P ₅ Cr ₇
Cr4	$3k$	$m..$	0.2044	0.3935	$\frac{1}{2}$		11-vertex polyhedron P ₅ Cr ₆
P5	$3k$	$m..$	0.269	0.09	$\frac{1}{2}$		square antiprism Cr ₈
Cr6	$3k$	$m..$	0.2893	0.2671	$\frac{1}{2}$		15-vertex Frank-Kasper P ₅ Cr ₁₀
Cr7	$3k$	$m..$	0.5114	0.3536	$\frac{1}{2}$		cuboctahedron P ₄ Cr ₆ Zr ₂
P8	$3k$	$m..$	0.5117	0.1961	$\frac{1}{2}$		trigonal prism Cr ₆
Cr9	$3j$	$m..$	0.025	0.2864	0		15-vertex Frank-Kasper P ₅ Cr ₁₀
Cr10	$3j$	$m..$	0.1585	0.5098	0		tetrahedron P ₄
P11	$3j$	$m..$	0.1742	0.2673	0		square antiprism Cr ₈
Cr12	$3j$	$m..$	0.1776	0.1094	0		cuboctahedron P ₄ Cr ₈
P13	$3j$	$m..$	0.318	0.5135	0		trigonal prism Cr ₆
Cr14	$3j$	$m..$	0.3938	0.1917	0		cuboctahedron P ₅ Cr ₇
P15	$3j$	$m..$	0.4134	0.3667	0		square antiprism Cr ₈
Cr16	$3j$	$m..$	0.4774	0.0643	0		cuboctahedron P ₅ Cr ₇
Zr17	$1e$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	0		23-vertex polyhedron P ₉ Cr ₁₂ Zr ₂
Zr18	$1d$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		23-vertex polyhedron P ₉ Cr ₁₂ Zr ₂
P19	$1a$	$-6..$	0	0	0		tricapped trigonal prism Cr ₉

Experimental: single crystal, diffractometer, X-rays, $R = 0.029$, $T = 295$ K

References: [1] Le Sénéchal C., Pivan J.Y., Députier S., Guérin R. (1998), Mater. Res. Bull. 33, 887-902.