

Cr_7C_3	$hP80$	(186) $P6_3mc - d^3c^7b$
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Cr_7C_3 [1]

Structural features: CCr_6Cr_3 tricapped trigonal prisms (non parallel prism axes) share atoms to form a 3D-framework.

Westgren A. (1935) [1]

C_3Cr_7

$a = 1.398$, $c = 0.4523$ nm, $c/a = 0.324$, $V = 0.7656$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cr1	12d	1	0.04	0.27	0.0		15-vertex Frank-Kasper C_4Cr_{11}
Cr2	12d	1	0.06	0.44	0.25		15-vertex Frank-Kasper C_4Cr_{11}
C3	12d	1	0.40	0.10	0.25		tricapped trigonal prism Cr_9
C4	6c	.m.	0.10	0.90	0.25		tricapped trigonal prism Cr_9
Cr5	6c	.m.	0.23	0.77	0.0		15-vertex Frank-Kasper C_4Cr_{11}
C6	6c	.m.	0.40	0.60	0.25		tricapped trigonal prism Cr_9
Cr7	6c	.m.	0.56	0.44	0.25		15-vertex Frank-Kasper C_4Cr_{11}
Cr8	6c	.m.	0.73	0.27	0.0		15-vertex Frank-Kasper C_4Cr_{11}
Cr9	6c	.m.	0.833	0.167	0.0		15-vertex Frank-Kasper C_3Cr_{12}
Cr10	6c	.m.	0.94	0.06	0.25		15-vertex Frank-Kasper C_4Cr_{11}
Cr11	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0		15-vertex Frank-Kasper C_3Cr_{12}

Transformation from published data: origin shift 0 0 0.75

Experimental: single crystal, rotation photographs, X-rays

Remarks: The authors state that true symmetry is space group (159) $P31c$. The structure was redetermined in space group (62) $Pnma$ in [2]; the authors state that the apparent hexagonal (or trigonal) symmetry is due to twinning. In [1] the z -coordinates of former Cr3, Cr4, Cr5 and C3 are misprinted as $\frac{3}{4}$, $\frac{1}{4}$, $\frac{3}{4}$ and $\frac{1}{2}$ instead of $\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{4}$ and 0, respectively (from the drawing in fig. 2)

References: [1] Westgren A. (1935), Jernkontorets Ann. 118, 231-240. [2] Rouault M.A., Herpin P., Fruchart M.R. (1970), Ann. Chim. (Paris) 5, 461-470.