

$\text{Er}_4(\text{Ga}_{0.19}\text{Ge}_{0.81})_7$	$hP11$	(187) $P\text{-}6m2 - k_j^2da$
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# **Er<sub>4</sub>(Ga,Ge)<sub>7</sub> [1]**

Structural features: 3D-framework of fused Er<sub>6</sub> trigonal prisms <sup>7</sup>/<sub>8</sub> of which are centered by (Ge,Ga); the empty prisms form columns parallel to [001]. Vacancy derivative of AlB<sub>2</sub>.

Venturini G. et al. (1999) [1]

Er<sub>4</sub>Ga<sub>1.33</sub>Ge<sub>5.67</sub>

$a = 0.7964$ ,  $c = 0.4095$  nm,  $c/a = 0.514$ ,  $V = 0.2249$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Er1	$3k$	$mm2$	0.83457	0.16543	$\frac{1}{2}$		pseudo Frank-Kasper Ge <sub>10</sub> Er <sub>8</sub>
M2	$3j$	$mm2$	0.17267	0.82733	0		tricapped trigonal prism Ge <sub>3</sub> Er <sub>6</sub>
M3	$3j$	$mm2$	0.52467	0.47533	0		10-vertex polyhedron Ge <sub>4</sub> Er <sub>6</sub>
Er4	$1d$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper Ge <sub>12</sub> Er <sub>8</sub>
M5	$1a$	$-6m2$	0	0	0		tricapped trigonal prism Ge <sub>3</sub> Er <sub>6</sub>

M2 = 0.81Ge + 0.19Ga; M3 = 0.81Ge + 0.19Ga; M5 = 0.81Ge + 0.19Ga

Transformation from published data:  $-x, -y, -z$ ; origin shift  $\frac{1}{3} \frac{2}{3} 0$

Experimental: powder, diffractometer, X-rays,  $R_p = 0.116$

Remarks: In table 4 of [1] the Wyckoff position of former Er<sub>1</sub> is misprinted as  $1f$  instead of  $1d$ .

References: [1] Venturini G., Vernière A., Malaman B. (1999), J. Alloys Compd. 291, 201-207.