

$\text{La}_{3.67}\text{FeC}_6$ $hP24$ $(176) P6_3/m - h^3ec$ **La_{3.67}FeC₆** [1]

Structural features: $\text{Fe}(\text{C}_2)_3$ trigonal units in La_6La_3 tricapped trigonal prisms, which share atoms to form a 3D-framework; additional La in channels of hexagonal cross-section parallel to [001] (partial disorder). C_2 pairs. Variant of $\text{Eu}_{3.16}\text{NiC}_6$.

Witte A.M., Jeitschko W. (1996) [1]

 $\text{C}_6\text{FeLa}_{3.67}$ $a = 0.8783$, $c = 0.5351$ nm, $c/a = 0.609$, $V = 0.3575$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	6h	$m..$	0.015	0.285	$\frac{1}{4}$		single atom C
C2	6h	$m..$	0.148	0.444	$\frac{1}{4}$		non-colinear CFe
La3	6h	$m..$	0.39623	0.33606	$\frac{1}{4}$		pentagonal bipyramid C ₇
La4	4e	3..	0	0	0.0674	0.333	
Fe5	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle C ₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.052$

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for site La4, refined value 0.320(3), set to $\frac{1}{3}$. Short interatomic distances for partly occupied site(s).

References: [1] Witte A.M., Jeitschko W. (1996), Z. Naturforsch. B 51, 249-256.