

KLaFe[CN]₆[H₂O]₄*hP*42(176) *P*6₃/*m* – i²hf²db**KLa[Fe(CN)₆]·4H₂O** [1]

Structural features: FeC₆ octahedra and LaN₆(OH₂)₃ tricapped trigonal prisms are interconnected via C-N bonds (cyanide units) to form a 3D-framework; K and additional H₂O between the units (substitutional disorder, distinct positions).

Beall G.W. et al. (1978) [1]

C₆FeH₈KLaN₆O₄*a* = 0.7412, *c* = 1.3943 nm, *c/a* = 1.881, *V* = 0.6634 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	12 <i>i</i>	1	0.2358	0.1655	0.0778		single atom N
N2	12 <i>i</i>	1	0.3813	0.2669	0.1241		single atom C
(OH ₂)3	6 <i>h</i>	<i>m</i> ..	0.071	0.4216	¹ / ₄		single atom La
(OH ₂)4	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0726	0.5	
K5	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0874	0.5	
La6	2 <i>d</i>	-6..	² / ₃	¹ / ₃	¹ / ₄		tricapped trigonal prism N ₆ (OH ₂) ₃
Fe7	2 <i>b</i>	-3..	0	0	0		octahedron C ₆

Transformation from published data: origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.030

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Beall G.W., Mullica D.F., Milligan W.O. (1978), Acta Crystallogr. B 34, 1446-1449.