$LaFe[CN]_6[H_2O]_5$	*hP*38	(176) $P6_3/m$ – i^2hfdb

$La[Fe(CN)_6]\cdot 5H_2O$ [2]
Structural features: FeC_6 octahedra and $LaN_6(OH_2)_3$ tricapped trigonal prisms are interconnected via C-N bonds (cyanide units) to form a 3D-framework; additional H_2O between the units. See Fig. IV.64.

Mullica D.F. et al. (1980) [1]
$C_6FeH_{10}LaN_6O_5$
$a = 0.7554$, $c = 1.4452$ nm, $c/a = 1.913$, $V = 0.7142$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
C1	12*i*	1	0.2401	0.1326	0.0769		single atom N
N2	12*i*	1	0.3843	0.2174	0.1228		single atom C
$(OH_2)3$	6*h*	*m*..	0.0614	0.4913	$^1/_4$		single atom La
$(OH_2)4$	4*f*	3..	$^1/_3$	$^2/_3$	0.0852		non-coplanar triangle $(OH_2)_3$
La5	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		tricapped trigonal prism $(OH_2)_3N_6$
Fe6	2*b*	-3..	0	0	0		octahedron C_6

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 290 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The description of a similar structure proposal for the tetrahydrate in space group (176) $P6_3/m$ in [1] does not take into consideration all symmetry elements; correct space group for the proposed structure is (194) $P6_3/mmc$ (see [3]), however, space group (63) *Cmcm* is generally preferred for tetrahydrates.

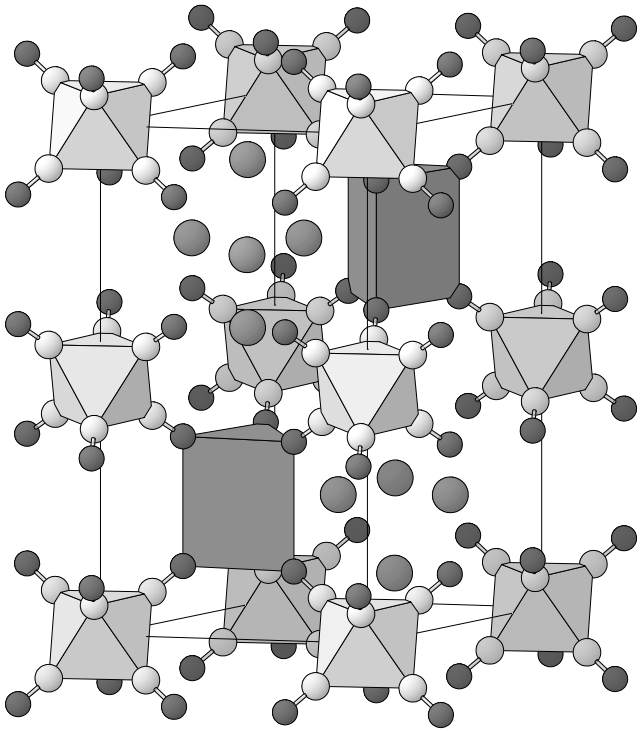

Fig. IV.64. **$LaFe(CN)_6\cdot 5H_2O$**

Arrangement of FeC_6 octahedra (C atoms light), LaN_6 trigonal prisms (N atoms dark) and H_2O molecules (O atoms large).

References: [1] Mullica D.F., Milligan W.O., Garner R.L. (1980), Acta Crystallogr. B 36, 2561-2564. [2] Bailey W.E., Williams R.J., Milligan W.O. (1973), Acta Crystallogr. B 29, 1365-1368. [3] Herbstein F.H., Marsh R.E. (1982), Acta Crystallogr. B 38, 1051-1055.