$Fe[NO]_3Cl$	*hP*16	(186) $P6_3mc - c^2b^2$

$Fe(NO)_3Cl$ [1]
Structural features: $Fe(NO)_3Cl$ tetrahedral units (a central $Fe(N_3Cl)$ tetrahedron, approximately linear Fe-N=O segments) in a Mg-type (h.c.p.) arrangement.

Hayton T.W. et al. (2003) [1]
$ClFeN_3O_3$
$a = 0.71701$, $c = 0.60403$ nm, $c/a = 0.842$, $V = 0.2689$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
N1	6*c*	.*m*.	0.7934	0.2065	0.39293		single atom O
O2	6*c*	.*m*.	0.8637	0.1363	0.26823		single atom N
Fe3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0		non-coplanar triangle N_3
Cl4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.37273		single atom Fe

Transformation from published data: origin shift 0 0 0.78987
Experimental: single crystal, diffractometer, X-rays, R = 0.024, T = 173 K

References: [1] Hayton T.W., McNeil W.S., Patrick B.O., Legzdins P. (2003), J. Am. Chem. Soc. 125, 12935-12944.