

$C[CN]_3Cl$	$hP48$	$(176) P6_3/m - i^2h^4$
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$CCl(CN)_3$ hexagonal [1]

Structural features: $C(CN)_3Cl$ tetrahedral molecules (a central $C(C_3Cl)$ tetrahedron with a N bonded to each C vertex, linear C-C-N segments).

Witt J.R. et al. (1972) [1]

C_4ClN_3

$a = 1.023$, $c = 0.995$ nm, $c/a = 0.973$, $V = 0.9018$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	$12i$	1	0.1298	0.3876	0.1347		non-colinear NC
N2	$12i$	1	0.2029	0.4201	0.0228		single atom C
C3	$6h$	$m..$	0.0363	0.35	$\frac{1}{4}$		tetrahedron C_3Cl
N4	$6h$	$m..$	0.2149	0.1598	$\frac{1}{4}$		single atom C
C5	$6h$	$m..$	0.2571	0.0749	$\frac{1}{4}$		non-colinear NC
Cl6	$6h$	$m..$	0.5146	0.0654	$\frac{1}{4}$		single atom C

Transformation from published data: $y, x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.088$

References: [1] Witt J.R., Britton D., Mahon C. (1972), Acta Crystallogr. B 28, 950-955.