$C_6Cl_3F_3$	*hP*24	(176) $P6_3/m$ – h^4

$C_6Cl_3F_3$ sym [1]
Structural features: Planar $C_6Cl_3F_3$ molecules (a C_6 hexagon with alternatively one Cl or F bonded to each C) in a Mg-type (h.c.p.) arrangement.

Chaplot S.L. et al. (1981) [1]
$C_6Cl_3F_3$
a = 0.8541, c = 0.6282 nm, c/a = 0.736, V = 0.3969 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	6*h*	*m*..	0.1446	0.525	$^1/_4$		coplanar triangle FC_2
Cl2	6*h*	*m*..	0.2278	0.2621	$^1/_4$		single atom C
C3	6*h*	*m*..	0.2855	0.4843	$^1/_4$		coplanar triangle C_2Cl
F4	6*h*	*m*..	0.4373	0.0195	$^1/_4$		single atom C

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.039

Remarks: 1,3,5-trichloro-2,4,6-trifluorobenzene, referred to as symmetric trichloro-trifluorobenzene. We derived conventional atom coordinates from the orthogonal coordinates reported in [1].

References: [1] Chaplot S.L., McIntyre G.J., Mierzejewski A., Pawley G.S. (1981), Acta Crystallogr. B 37, 1896-1900.