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Dichlorobis(2,4-dichloro-5-fluorophenyl)-methane

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The molecule of the title compound, $C_{13}H_4Cl_6F_2$, has twofold crystallographic symmetry, with the axis passing through the central methlyene C atom. The dihedral angle between the two aromatic residues is 86.13 (8)°.

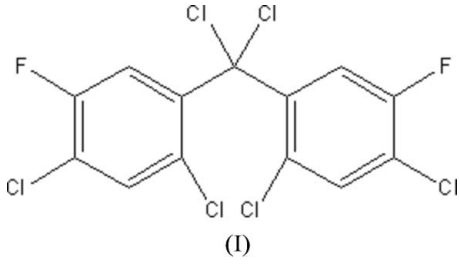
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.088
Data-to-parameter ratio = 12.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Bis(2,4-dichloro-5-fluorophenyl)dichloromethane, (I), is an important intermediate in organic synthesis (Kumai *et al.*, 1991) and was obtained from the reaction of CCl_4 and 1,3-dichloro-4-fluorobenzene, as colorless crystals suitable for X-ray crystallographic analysis.



(I)

The molecule of (I) has twofold crystallographic symmetry (Fig. 1) with the axis passing through the methylene atom C7. The dihedral angle between the two aromatic residues is 86.13 (8)°.

Experimental

Compound (I) was prepared according to the procedure of Kumai *et al.* (1991). A solution of (I) in methanol was concentrated gradually at room temperature to afford colorless blocks.

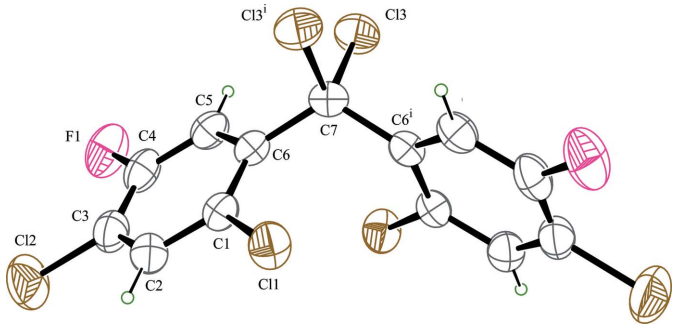


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are shown at the 30% probability level. [Symmetry code: (i) $x, \frac{1}{2}-y, \frac{1}{2}-z$.]

Crystal data

$C_{13}H_4Cl_6F_2$	$Z = 4$
$M_r = 410.89$	$D_x = 1.806$ Mg m^{-3}
Orthorhombic, *Pnna*	Mo $K\alpha$ radiation
$a = 19.896$ (9) Å	$\mu = 1.14$ mm^{-1}
$b = 11.483$ (4) Å	$T = 298$ (1) K
$c = 6.614$ (2) Å	Block, colorless
$V = 1510.9$ (10) Å^3	0.43 × 0.33 × 0.30 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	13211 measured reflections
	1734 independent reflections
ω scans	1186 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.037$
	$\theta_{max} = 27.5^\circ$
$T_{min} = 0.613$, $T_{max} = 0.710$	

Refinement

Refinement on F^2	$w = 1/[0.0007F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.088$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
1189 reflections	Extinction correction: Larson (1970), equation 22
97 parameters	
H-atom parameters constrained	Extinction coefficient: 40 (2)

The H atoms were included in the riding-model approximation with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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