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2,4-Bis[2-chloro-4-(trifluoromethyl)phenoxy]-1-nitrobenzene

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.051
wR factor = 0.164
Data-to-parameter ratio = 13.2

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

The title compound, $C_{20}H_9Cl_2F_6NO_4$, a member of the class of nitrophenyl ether herbicides, features two ether O atoms that link two trifluoromethyl-substituted aromatic rings to a central aromatic ring. The molecules are linked by an F···F interaction into a linear chain.

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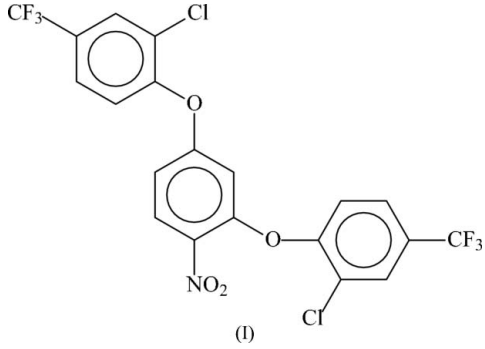
Comment

This study of the title compound, (I), follows a similiar study of the class of nitrophenyl ether herbicides (Gao & Ng, 2005).



(I)

The central nitrophenylene group of (I) is connected to two trifluoromethyl-substituted aromatic rings (Fig. 1). The ring

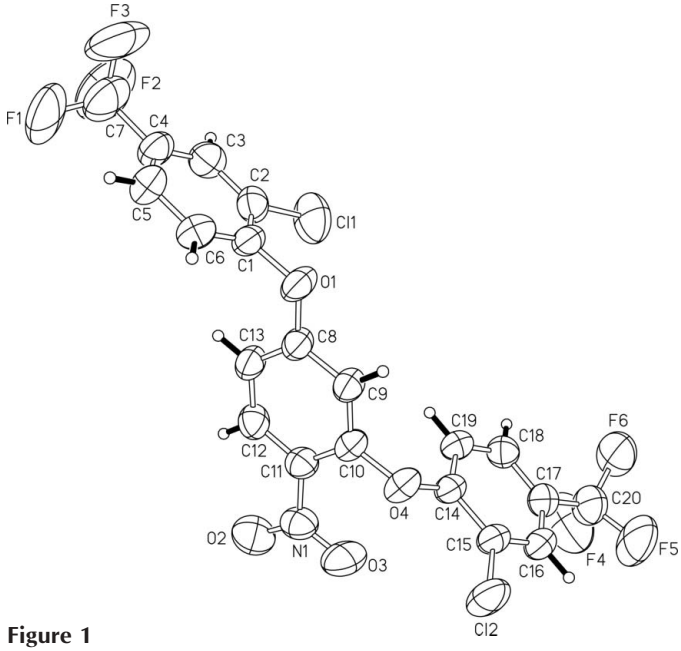


Figure 1
A plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. For each CF^3 group only one disorder component is shown.

para to the nitro group is twisted by 83.7 (1)° relative to the central ring, whereas the ring *ortho* to it is twisted by 87.9 (1)°.

F···F interactions [F1···F2^{i} = 2.71 (1) Å; symmetry code: (i) $2-x, y-\frac{1}{2}, \frac{3}{2}-z$] link adjacent molecules into a linear chain (Fig. 2).

Experimental

The title compound was purchased from Tianjian Bodi Chemical Reagent Company and was recrystallized from ethanol.

Crystal data

$C_{20}H_9Cl_2F_6NO_4$	D_x = 1.658 Mg m^{-3}
M_r = 512.18	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 15755 reflections
a = 17.056 (3) Å	θ = 3.1–27.5°
b = 9.074 (2) Å	μ = 0.40 mm^{-1}
c = 13.544 (3) Å	T = 295 (2) K
β = 101.88 (3)°	Prism, colourless
V = 2051.5 (7) Å^3	0.39 × 0.25 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS-RAPID IP diffractometer	4666 independent reflections
	3310 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.022
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	θ_{max} = 27.5°
	$h = -22 \rightarrow 21$
T_{min} = 0.519, T_{max} = 0.928	$k = -11 \rightarrow 11$
18242 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 0.4142P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.051	
$wR(F^2)$ = 0.164	
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
4666 reflections	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
354 parameters	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
H-atom parameters constrained	

The two trifluoromethyl groups are disordered over two positions, and they were refined with restraints. In each group, the six C—F distances were restrained to within 0.01 (1) Å of each other, as were the F···F interactions. The six F atoms were restrained to lie in a plane, and their vibrations were restrained to be nearly isotropic. The site occupancies refined to 50 (1):50 (1) for F1/F2/F3 and 54 (1):46 (1) for F4/F5/F6. H atoms were positioned geometrically, with C—H = 0.93 Å, and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *RAPID AUTO* (Rigaku, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

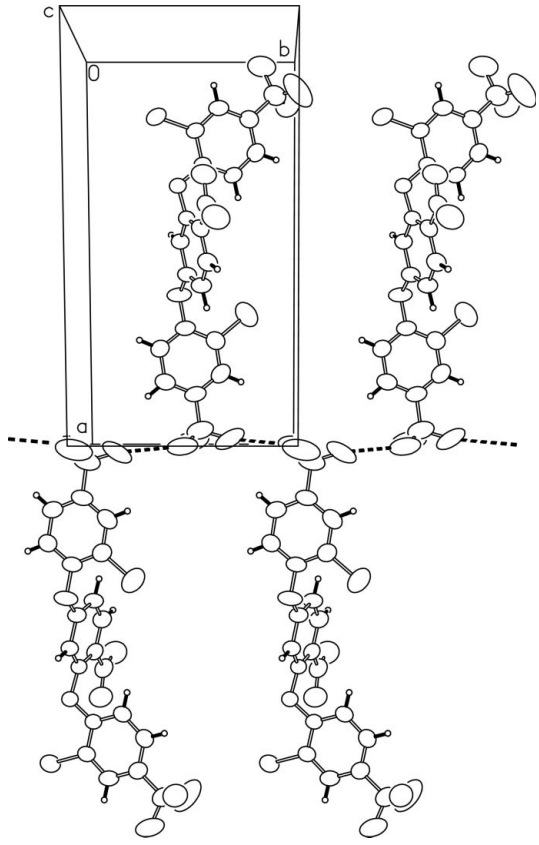


Figure 2
Diagram showing the chain structure arising from the F···F interactions.

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