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2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene

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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 = 0.050
wR factor = 0.157
Data-to-parameter ratio = 13.7

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

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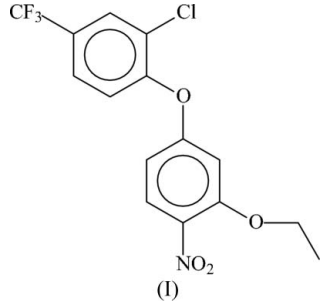
The title compound, $C_{15}H_{11}ClF_3NO_4$, a member of the class of nitrophenyl ether herbicides, features an ether O atom that links two substituted aromatic rings, the rings being twisted from each other by 62.5 (1)°. The two ether C—O distances are statistically indistinguishable from each other, despite the different nature of the electron-withdrawing groups in the 4-position (relative to the ether linkage).

Comment

2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-trifluoromethylbenzene, (I) (Fig. 1), belongs to a class of nitrophenyl ether herbicides marketed under the trade names Goal, Point, Cavalier and Striker. It is also known as oxyfluorfen. The structure of the compound has been investigated by quantum-chemical calculations (Gu, 1999). The structure–activity relationship of this and other O-bridged protoporphyrinogen oxidase inhibitors has also been examined by QSAR modelling (Dayan *et al.*, 1999; Nandihalli *et al.*, 1992). The compound exhibits photo-bleaching behaviour, which is explained in terms of its lowest unoccupied molecular orbital (LUMO; Akagi & Skashita, 1993). The present solid-state structure complements these studies.



(I)

Compound (I) exists as a monomeric molecule having two substituted aromatic rings connected through an ether linkage. The rings are twisted by 62.5 (1)° in order to avoid steric congestion by the 2-chloro substituent in one ring. The two ether C—O distances are statistically indistinguishable from each other, despite the different nature of the electron-withdrawing groups in the 4-position (relative to the ether linkage). The bonds are, however, much longer than the ethoxy C—O bond in the molecule.

Experimental

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

Crystal data

$C_{15}H_{11}ClF_3NO_4$	D_x = 1.521 Mg m^{-3}
M_r = 361.70	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 13669 reflections
a = 29.140 (6) Å	θ = 3.0–27.5°
b = 7.646 (2) Å	μ = 0.29 mm^{-1}
c = 14.511 (3) Å	T = 295 (2) K
β = 102.19 (3)°	Block, colourless
V = 3160 (1) Å^3	0.37 × 0.28 × 0.21 mm
Z = 8	

Data collection

Rigaku R-AXIS-RAPID IP diffractometer	3600 independent reflections
ω scans	2486 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.019
T_{min} = 0.746, T_{max} = 0.941	θ_{max} = 27.5°
14665 measured reflections	$h = -33 \rightarrow 37$
	$k = -8 \rightarrow 9$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0871P)^2 + 0.6851P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.157	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
S = 1.09	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
3600 reflections	
262 parameters	
H-atom parameters constrained	

The trifluromethyl group is disordered over two sites; the six C—F bond distances were restrained to within 0.01 Å of each other, as were the F···F distances. The six F atoms were restrained to lie in a plane. As the disorder refined to nearly 50:50, the disorder was fixed as exactly 50:50. The nitro group is also disordered over two sites; the four N—O bond distances were restrained to within 0.01 Å of each other, as were the O···O distances. Atom C11 and the three atoms of the nitro group were restrained to lie in a plane for both components. The disorder refined to nearly 50:50; however, the occupancy was fixed at exactly 50:50 so that the primed nitro group of one molecule is not close to the primed nitro group of the adjacent one. The disordered F and O atoms were restrained to behave in a nearly isotropic manner. H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for the methylene H atoms, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl H atoms.

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*.

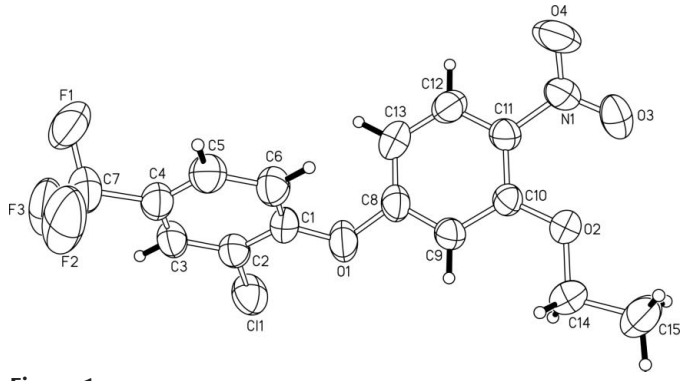


Figure 1
A plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Only one set of the disordered atoms is shown.

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