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1,3,4,4-Tetrachloro-4-(4-chlorophenylsulfanyl)-2-nitrobuta-1,3-diene

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Key indicators

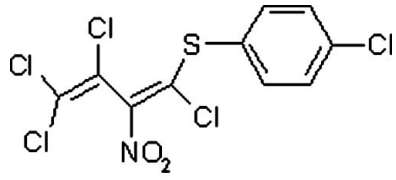
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.079
wR factor = 0.085
Data-to-parameter ratio = 19.6

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

The molecule of the title compound, $C_{10}H_4Cl_5NO_2S$, is not planar. The chlorophenyl ring and the butadiene group are inclined at an angle of 59.5 (1)°.

Comment

The chemistry of nitro compounds, especially their halogen derivatives, has been intensively studied in recent decades. These highly reactive subtances have been used to develop preparative methods for the synthesis of complex polyfunctional derivatives of different classes. However, there are only a few reports on the crystal structures of halogened nitrobutadiene compounds. The title compound, (I), was synthesized from 2-nitropentachlorobutadiene and *p*-chlorothiophenol (Ibis & Goksel, 1994). Crystallographic analysis was carried out and the results are presented in this paper.



(I)

The molecule is not planar. The chlorophenyl ring and the butadiene group are inclined at an angle of 59.5 (1)°. The C—C bond lengths of the butadiene chain agree well with corresponding distances in a similar compound (Surange *et al.*, 1997).

Experimental

p-Chlorothiophenol (1.06 g, 7.37 mmol) and 2-nitropentachloro-1,3-butadiene (2 g, 7.37 mmol) were stirred for 24 h at room temperature. The product was extracted with chloroform; the organic layer was separated and washed with distilled water (3 × 30 ml) and dried with Na_2SO_4. The solvent was evaporated and the residue was purified by cystallization from ethanol (yield: 2.2 g, 79%; m.p. 386–388 K).

Crystal data

$C_{10}H_4Cl_5NO_2S$
M_r = 379.46
Triclinic, $P\overline{1}$
a = 6.6504 (4) Å
b = 10.7872 (3) Å
c = 10.857 (4) Å
α = 70.481 (4)°
β = 87.411 (8)°
γ = 83.680 (7)°
V = 729.6 (3) Å^3
Z = 2
D_x = 1.727 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6436 reflections
θ = 3.1–30.1°
μ = 1.13 mm^{-1}
T = 293.5 K
Block, yellow
0.40 × 0.30 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	4303 independent reflections
ω scans	3450 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.021$
$T_{min} = 0.677$, $T_{max} = 0.760$	$\theta_{max} = 30.1^\circ$
8204 measured reflections	$h = -9 \rightarrow 9$
	$k = -14 \rightarrow 15$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F	Chebychev polynomial with three parameters (Carruthers & Watkin, 1979): 9.9084, 2.2048 and 6.4348
$R[F^2 > 2\sigma(F^2)] = 0.079$	$(\Delta/\sigma)_{max} = 0.009$
$wR(F^2) = 0.085$	$\Delta\rho_{max} = 1.24$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.77$ e Å^{-3}
3450 reflections	
176 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.285 (8)	C3—C4	1.354 (5)
C2—C3	1.478 (5)		
C3—C2—C1	122.8 (4)	C4—C3—C2	125.1 (4)

H atoms were treated as riding, with C—H = 0.95 (6) Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum electron-density peak is located 0.62 Å from atom Cl3.

Data collection: *CRYSTALCLEAR* (Rigaku/MSC, 2002); cell refinement: *CRYSTALCLEAR*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

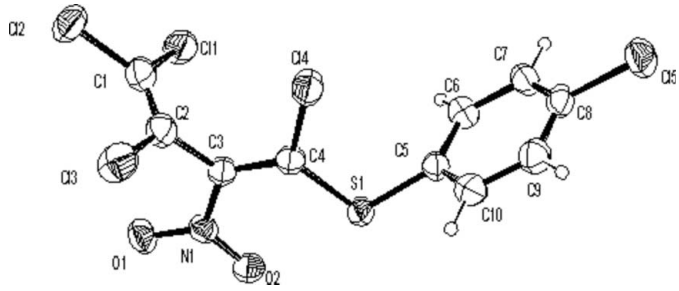


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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