

2-Nitro-*p*-phenylene bis(toluene-sulfonate)

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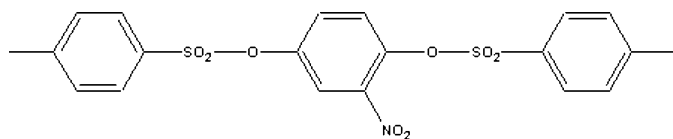
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 6.8.

In the molecule of the title compound, $\text{C}_{20}\text{H}_{17}\text{NO}_8\text{S}_2$, the two toluene rings are oriented at a dihedral angle of $3.65(4)^\circ$, while the nitrophenyl ring is oriented at dihedral angles of $44.39(3)$ and $47.44(3)^\circ$ with respect to the toluene rings. An intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond results in the formation of a five-membered ring, which adopts an envelope conformation. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules. There is a $\pi-\pi$ contact between the toluene rings [centroid-centroid distance = $4.035(1)$ Å].

Related literature

For related literature, see: Atkinson *et al.* (2005); Hu *et al.* (2001); Svensson *et al.* (1998); Trollsås *et al.* (1996). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{17}\text{NO}_8\text{S}_2$
 $M_r = 463.49$

 Triclinic, $P1$
 $a = 7.926(3)$ Å

 $b = 8.244(3)$ Å

 $c = 8.709(3)$ Å

 $\alpha = 98.323(6)^\circ$
 $\beta = 96.180(6)^\circ$
 $\gamma = 103.915(6)^\circ$
 $V = 540.5(3)$ Å³
 $Z = 1$

 Mo $K\alpha$ radiation

 $\mu = 0.29$ mm⁻¹
 $T = 294(2)$ K

 $0.26 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

 $T_{\min} = 0.928$, $T_{\max} = 0.955$

2693 measured reflections

1918 independent reflections

 1717 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.135$
 $S = 1.05$

1918 reflections

282 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Absolute structure: Flack (1983),

315 Friedel Pairs

Flack parameter: 0.21 (13)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{i}}$	0.93	2.49	3.405 (11)	168
$\text{C9}-\text{H9}\cdots\text{O6}^{\text{ii}}$	0.93	2.46	3.319 (9)	153
$\text{C10}-\text{H10}\cdots\text{O8}^{\text{i}}$	0.93	2.47	3.369 (10)	164
$\text{C11}-\text{H11}\cdots\text{O1}^{\text{iii}}$	0.93	2.50	3.352 (10)	153
$\text{C15}-\text{H15}\cdots\text{O5}$	0.93	2.56	2.923 (10)	104
$\text{C18}-\text{H18}\cdots\text{O5}^{\text{iv}}$	0.93	2.49	3.409 (11)	168

 Symmetry codes: (i) $x, y + 1, z$; (ii) $x, y, z + 1$; (iii) $x, y, z - 1$; (iv) $x, y - 1, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2500).

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supplementary materials

Acta Cryst. (2008). E64, o1816 [doi:10.1107/S1600536808026573]

2-Nitro-*p*-phenylene bis(toluenesulfonate)

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Comment

Phenolic esters are useful intermediates in organic synthesis (Trollsås *et al.*, 1996; Svensson *et al.*, 1998; Atkinson *et al.*, 2005; Hu *et al.*, 2001). We have developed a new method for the syntheses of some phenolic esters. The title compound has been produced as a byproduct. We report herein its crystal structure.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C1—C6), B (C8—C13) and C (C14—C19) are, of course, planar, and the dihedral angles between them are A/B = 44.39 (3)°, A/C = 3.65 (4)° and B/C = 47.44 (3)°. The intramolecular C—H···O hydrogen bond (Table 1) results in the formation of a five-membered ring D (S2/O5/C14/C15/H15), adopting envelope conformation, with O5 atom displaced by 0.356 (3) Å from the plane of the other ring atoms.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure. A π — π contact between A and C rings $Cg1 \cdots Cg3^i$ [symmetry code: (i) $1 + x, 1 + y, 1 + z$, where $Cg1$ and $Cg3$ are the centroids of the rings A and C, respectively] further stabilize the structure, with centroid-centroid distance of 4.035 (1) Å.

Experimental

For the preparation of the title compound, 2-nitrohydroquinone (155 mg, 1.0 mmol) was dissolved in chloroform (30 ml). To this solution, 4-toluenesulfonyl chloride (191 mg, 1.0 mmol) and triethylamine (101 mg, 1.0 mmol) were added, the reaction was stirred at room temperature for 3 h. The reaction mixture was extracted with dichloromethane and dried with anhydrous sodium sulfate. After concentration, the residue was separated by flash column chromatography and purified by recrystallization from chloroform (yield; 72 mg, 31%, m.p. 415 K). Spectroscopic analysis: IR (KBr, ν , cm^{-1}): 3089, 2922, 1596, 1539, 1390, 1201, 1183, 1089. Analysis required for $\text{C}_{20}\text{H}_{17}\text{NO}_8\text{S}_2$: C 51.83; H 3.70; N 3.02%. Found: C 50.85; H 3.65; N 3.19%.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H atoms.

Figures

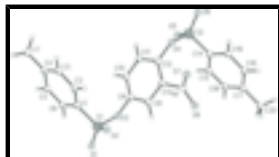


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

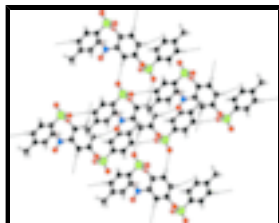


Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

2-Nitro-p-phenylene bis(toluenesulfonate)

Crystal data

$C_{20}H_{17}NO_8S_2$

$M_r = 463.49$

Triclinic, $P1$

Hall symbol: $P1$

$a = 7.926 (3) \text{ \AA}$

$b = 8.244 (3) \text{ \AA}$

$c = 8.709 (3) \text{ \AA}$

$\alpha = 98.323 (6)^\circ$

$\beta = 96.180 (6)^\circ$

$\gamma = 103.915 (6)^\circ$

$V = 540.5 (3) \text{ \AA}^3$

$Z = 1$

$F_{000} = 240$

$D_x = 1.424 \text{ Mg m}^{-3}$

Melting point: 415 K

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1246 reflections

$\theta = 2.6\text{--}26.9^\circ$

$\mu = 0.29 \text{ mm}^{-1}$

$T = 294 (2) \text{ K}$

Block, colorless

$0.26 \times 0.22 \times 0.16 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2) \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.928$, $T_{\max} = 0.955$

2693 measured reflections

1918 independent reflections

1717 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 2.4^\circ$

$h = -9 \rightarrow 6$

$k = -7 \rightarrow 9$

$l = -10 \rightarrow 8$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0884P)^2 + 0.0596P]$
$wR(F^2) = 0.135$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\max} = 0.007$
1918 reflections	$\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$
282 parameters	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), with 315 Friedel Pairs
	Flack parameter: 0.21 (13)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.2533 (2)	0.96499 (17)	1.25707 (16)	0.0455 (6)
S2	-0.0820 (2)	0.52158 (16)	0.40141 (16)	0.0461 (6)
O1	0.1899 (10)	1.0093 (7)	1.3993 (6)	0.0661 (19)
O2	0.3449 (8)	0.8397 (6)	1.2462 (6)	0.0602 (18)
O3	0.0766 (7)	0.8988 (6)	1.1351 (6)	0.0461 (14)
O4	0.0995 (7)	0.5877 (7)	0.5288 (6)	0.0477 (15)
O5	-0.1792 (8)	0.6481 (6)	0.4198 (6)	0.0602 (17)
O6	-0.0204 (8)	0.4733 (7)	0.2588 (6)	0.0578 (16)
O7	0.2194 (9)	0.3656 (8)	0.7024 (7)	0.103 (2)
O8	0.0174 (10)	0.3014 (7)	0.8493 (7)	0.104 (2)
N1	0.1160 (10)	0.4007 (7)	0.7819 (7)	0.0713 (17)
C1	0.3630 (12)	1.1486 (10)	1.1911 (10)	0.043 (2)
C2	0.4931 (12)	1.1343 (12)	1.0940 (10)	0.058 (3)
H2	0.5251	1.0333	1.0693	0.069*
C3	0.5700 (14)	1.2794 (13)	1.0380 (11)	0.066 (3)
H3	0.6527	1.2728	0.9709	0.080*
C4	0.5312 (14)	1.4300 (14)	1.0756 (12)	0.063 (3)

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C5	0.4075 (13)	1.4426 (12)	1.1802 (12)	0.068 (3)
H5	0.3828	1.5461	1.2115	0.082*
C6	0.3232 (12)	1.2979 (11)	1.2355 (10)	0.055 (3)
H6	0.2402	1.3040	1.3025	0.066*
C7	0.6108 (16)	1.5928 (14)	1.0174 (12)	0.100 (4)
H7A	0.7225	1.6490	1.0800	0.150*
H7B	0.5334	1.6661	1.0256	0.150*
H7C	0.6267	1.5659	0.9098	0.150*
C8	0.0860 (11)	0.8191 (9)	0.9787 (8)	0.039 (2)
C9	0.0942 (10)	0.6546 (8)	0.9560 (9)	0.0405 (19)
H9	0.0989	0.5959	1.0392	0.049*
C10	0.0717 (12)	0.9097 (10)	0.8580 (9)	0.049 (2)
H10	0.0579	1.0193	0.8773	0.058*
C11	0.0786 (11)	0.8330 (9)	0.7098 (9)	0.050 (2)
H11	0.0740	0.8936	0.6279	0.060*
C12	0.0926 (10)	0.6654 (10)	0.6776 (9)	0.040 (2)
C13	0.0952 (10)	0.5776 (9)	0.8033 (9)	0.041 (2)
C14	-0.1986 (12)	0.3410 (11)	0.4653 (9)	0.039 (2)
C15	-0.3270 (10)	0.3498 (10)	0.5546 (9)	0.046 (2)
H15	-0.3577	0.4514	0.5797	0.055*
C16	-0.4131 (12)	0.2048 (11)	0.6089 (10)	0.051 (2)
H16	-0.5036	0.2094	0.6679	0.061*
C17	-0.3648 (13)	0.0550 (12)	0.5756 (10)	0.054 (3)
C18	-0.2358 (13)	0.0481 (11)	0.4832 (11)	0.059 (3)
H18	-0.2063	-0.0540	0.4571	0.071*
C19	-0.1494 (11)	0.1887 (10)	0.4286 (10)	0.053 (3)
H19	-0.0600	0.1833	0.3686	0.064*
C20	-0.4603 (13)	-0.1022 (13)	0.6365 (12)	0.082 (3)
H20A	-0.5067	-0.1946	0.5501	0.123*
H20B	-0.5548	-0.0775	0.6878	0.123*
H20C	-0.3792	-0.1331	0.7097	0.123*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0547 (15)	0.0356 (11)	0.0427 (13)	0.0047 (10)	0.0065 (11)	0.0075 (9)
S2	0.0554 (15)	0.0371 (12)	0.0423 (13)	0.0051 (10)	0.0035 (11)	0.0100 (9)
O1	0.097 (6)	0.056 (4)	0.043 (4)	0.009 (4)	0.017 (4)	0.012 (3)
O2	0.071 (5)	0.042 (4)	0.067 (4)	0.017 (3)	-0.001 (4)	0.016 (3)
O3	0.049 (4)	0.043 (3)	0.042 (3)	0.007 (3)	0.007 (3)	0.000 (2)
O4	0.046 (4)	0.048 (3)	0.044 (4)	0.000 (3)	0.011 (3)	0.008 (2)
O5	0.065 (5)	0.039 (4)	0.070 (4)	0.009 (3)	-0.004 (4)	0.009 (3)
O6	0.071 (5)	0.058 (4)	0.038 (4)	-0.002 (3)	0.014 (3)	0.013 (3)
O7	0.127 (5)	0.102 (5)	0.103 (4)	0.080 (4)	0.018 (4)	0.004 (3)
O8	0.169 (6)	0.043 (3)	0.103 (4)	0.029 (3)	0.009 (4)	0.031 (3)
N1	0.099 (5)	0.050 (3)	0.062 (3)	0.029 (3)	-0.016 (3)	0.003 (3)
C1	0.041 (6)	0.034 (5)	0.048 (6)	-0.001 (4)	0.003 (4)	0.006 (4)
C2	0.062 (7)	0.067 (6)	0.050 (5)	0.018 (5)	0.026 (5)	0.009 (4)

C3	0.063 (7)	0.075 (8)	0.055 (6)	0.000 (5)	0.017 (5)	0.016 (5)
C4	0.049 (7)	0.066 (7)	0.066 (7)	-0.004 (5)	-0.007 (5)	0.033 (5)
C5	0.054 (7)	0.043 (6)	0.106 (10)	0.006 (5)	0.005 (7)	0.024 (5)
C6	0.057 (7)	0.040 (5)	0.074 (7)	0.021 (5)	0.013 (5)	0.014 (4)
C7	0.085 (8)	0.093 (9)	0.099 (9)	-0.031 (7)	-0.006 (7)	0.048 (6)
C8	0.039 (5)	0.032 (4)	0.040 (5)	-0.002 (4)	0.006 (4)	0.008 (3)
C9	0.049 (6)	0.030 (4)	0.042 (5)	0.007 (4)	0.003 (4)	0.013 (3)
C10	0.060 (7)	0.028 (5)	0.050 (6)	0.005 (4)	-0.008 (5)	0.005 (4)
C11	0.056 (6)	0.041 (5)	0.046 (6)	-0.004 (4)	-0.003 (4)	0.020 (4)
C12	0.029 (5)	0.040 (5)	0.047 (6)	0.002 (4)	0.001 (4)	0.011 (4)
C13	0.041 (5)	0.033 (5)	0.050 (6)	0.008 (4)	0.006 (4)	0.013 (3)
C14	0.039 (5)	0.043 (5)	0.034 (5)	0.011 (4)	0.003 (4)	0.008 (4)
C15	0.040 (5)	0.036 (5)	0.056 (5)	0.006 (4)	-0.002 (4)	0.002 (3)
C16	0.040 (5)	0.070 (6)	0.047 (5)	0.014 (5)	0.012 (4)	0.018 (4)
C17	0.042 (6)	0.052 (6)	0.062 (6)	-0.004 (5)	0.004 (5)	0.018 (5)
C18	0.058 (7)	0.042 (5)	0.082 (7)	0.016 (5)	0.014 (6)	0.018 (5)
C19	0.048 (6)	0.043 (5)	0.067 (7)	0.004 (4)	0.025 (5)	0.008 (4)
C20	0.064 (7)	0.083 (8)	0.112 (9)	0.011 (6)	0.021 (6)	0.061 (6)

Geometric parameters (Å, °)

S1—O2	1.396 (6)	C7—H7B	0.9600
S1—O1	1.419 (6)	C7—H7C	0.9600
S1—O3	1.591 (6)	C8—C9	1.360 (9)
S1—C1	1.762 (8)	C8—C10	1.385 (10)
S2—O6	1.422 (5)	C9—C13	1.389 (9)
S2—O5	1.439 (6)	C9—H9	0.9300
S2—O4	1.643 (6)	C10—C11	1.366 (10)
S2—C14	1.752 (9)	C10—H10	0.9300
O3—C8	1.441 (8)	C11—C12	1.403 (10)
O4—C12	1.373 (8)	C11—H11	0.9300
O7—N1	1.189 (7)	C12—C13	1.398 (10)
O8—N1	1.247 (8)	C14—C15	1.355 (10)
N1—C13	1.494 (9)	C14—C19	1.405 (10)
C1—C6	1.357 (10)	C15—C16	1.400 (12)
C1—C2	1.417 (10)	C15—H15	0.9300
C2—C3	1.387 (13)	C16—C17	1.380 (12)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.353 (13)	C17—C18	1.374 (11)
C3—H3	0.9300	C17—C20	1.532 (12)
C4—C5	1.419 (13)	C18—C19	1.374 (12)
C4—C7	1.521 (14)	C18—H18	0.9300
C5—C6	1.399 (13)	C19—H19	0.9300
C5—H5	0.9300	C20—H20A	0.9600
C6—H6	0.9300	C20—H20B	0.9600
C7—H7A	0.9600	C20—H20C	0.9600
O2—S1—O1	119.0 (4)	C9—C8—O3	118.2 (6)
O2—S1—O3	108.4 (3)	C10—C8—O3	118.1 (7)
O1—S1—O3	102.0 (4)	C8—C9—C13	117.3 (7)

supplementary materials

O2—S1—C1	112.4 (4)	C8—C9—H9	121.3
O1—S1—C1	110.6 (4)	C13—C9—H9	121.3
O3—S1—C1	102.5 (4)	C11—C10—C8	117.9 (8)
O6—S2—O5	122.6 (4)	C11—C10—H10	121.0
O6—S2—O4	102.9 (3)	C8—C10—H10	121.0
O5—S2—O4	108.1 (3)	C10—C11—C12	121.8 (7)
O6—S2—C14	110.0 (4)	C10—C11—H11	119.1
O5—S2—C14	108.1 (4)	C12—C11—H11	119.1
O4—S2—C14	103.4 (4)	O4—C12—C13	120.7 (7)
C8—O3—S1	118.2 (5)	O4—C12—C11	122.0 (7)
C12—O4—S2	119.0 (5)	C13—C12—C11	117.3 (7)
O7—N1—O8	125.9 (6)	C9—C13—C12	121.9 (7)
O7—N1—C13	119.0 (7)	C9—C13—N1	116.6 (6)
O8—N1—C13	115.1 (6)	C12—C13—N1	121.2 (7)
C6—C1—C2	122.3 (9)	C15—C14—C19	120.7 (8)
C6—C1—S1	119.7 (7)	C15—C14—S2	120.8 (6)
C2—C1—S1	118.0 (6)	C19—C14—S2	118.4 (7)
C3—C2—C1	116.2 (8)	C14—C15—C16	119.5 (8)
C3—C2—H2	121.9	C14—C15—H15	120.3
C1—C2—H2	121.9	C16—C15—H15	120.3
C4—C3—C2	123.6 (10)	C17—C16—C15	120.4 (8)
C4—C3—H3	118.2	C17—C16—H16	119.8
C2—C3—H3	118.2	C15—C16—H16	119.8
C3—C4—C5	118.8 (10)	C18—C17—C16	119.2 (9)
C3—C4—C7	125.8 (12)	C18—C17—C20	121.1 (9)
C5—C4—C7	115.3 (11)	C16—C17—C20	119.7 (9)
C6—C5—C4	119.3 (9)	C17—C18—C19	121.4 (9)
C6—C5—H5	120.3	C17—C18—H18	119.3
C4—C5—H5	120.3	C19—C18—H18	119.3
C1—C6—C5	119.6 (9)	C18—C19—C14	118.7 (8)
C1—C6—H6	120.2	C18—C19—H19	120.6
C5—C6—H6	120.2	C14—C19—H19	120.6
C4—C7—H7A	109.5	C17—C20—H20A	109.5
C4—C7—H7B	109.5	C17—C20—H20B	109.5
H7A—C7—H7B	109.5	H20A—C20—H20B	109.5
C4—C7—H7C	109.5	C17—C20—H20C	109.5
H7A—C7—H7C	109.5	H20A—C20—H20C	109.5
H7B—C7—H7C	109.5	H20B—C20—H20C	109.5
C9—C8—C10	123.5 (7)		
O2—S1—O3—C8	-45.0 (6)	S2—O4—C12—C11	-75.6 (9)
O1—S1—O3—C8	-171.4 (5)	C10—C11—C12—O4	179.9 (7)
C1—S1—O3—C8	74.1 (5)	C10—C11—C12—C13	1.4 (12)
O6—S2—O4—C12	171.7 (5)	C8—C9—C13—C12	1.6 (10)
O5—S2—O4—C12	40.7 (6)	C8—C9—C13—N1	176.1 (8)
C14—S2—O4—C12	-73.8 (6)	O4—C12—C13—C9	177.9 (6)
O2—S1—C1—C6	-160.2 (7)	C11—C12—C13—C9	-3.6 (11)
O1—S1—C1—C6	-24.6 (9)	O4—C12—C13—N1	3.6 (12)
O3—S1—C1—C6	83.5 (7)	C11—C12—C13—N1	-177.8 (7)
O2—S1—C1—C2	18.8 (9)	O7—N1—C13—C9	-132.7 (7)

O1—S1—C1—C2	154.4 (8)	O8—N1—C13—C9	48.5 (9)
O3—S1—C1—C2	-97.4 (8)	O7—N1—C13—C12	41.8 (11)
C6—C1—C2—C3	-4.1 (15)	O8—N1—C13—C12	-136.9 (8)
S1—C1—C2—C3	176.8 (7)	O6—S2—C14—C15	-152.6 (7)
C1—C2—C3—C4	2.3 (16)	O5—S2—C14—C15	-16.4 (9)
C2—C3—C4—C5	1.1 (17)	O4—S2—C14—C15	98.0 (8)
C2—C3—C4—C7	-179.8 (9)	O6—S2—C14—C19	30.7 (8)
C3—C4—C5—C6	-3.0 (16)	O5—S2—C14—C19	166.9 (6)
C7—C4—C5—C6	177.8 (8)	O4—S2—C14—C19	-78.6 (6)
C2—C1—C6—C5	2.4 (14)	C19—C14—C15—C16	-0.9 (13)
S1—C1—C6—C5	-178.6 (8)	S2—C14—C15—C16	-177.5 (6)
C4—C5—C6—C1	1.2 (14)	C14—C15—C16—C17	1.8 (13)
S1—O3—C8—C9	79.1 (8)	C15—C16—C17—C18	-2.6 (14)
S1—O3—C8—C10	-106.1 (8)	C15—C16—C17—C20	179.8 (9)
C10—C8—C9—C13	2.7 (12)	C16—C17—C18—C19	2.6 (15)
O3—C8—C9—C13	177.2 (7)	C20—C17—C18—C19	-179.8 (8)
C9—C8—C10—C11	-4.7 (13)	C17—C18—C19—C14	-1.8 (14)
O3—C8—C10—C11	-179.3 (7)	C15—C14—C19—C18	1.0 (12)
C8—C10—C11—C12	2.5 (12)	S2—C14—C19—C18	177.6 (7)
S2—O4—C12—C13	102.9 (8)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H5...O2 ⁱ	0.93	2.49	3.405 (11)	168
C9—H9...O6 ⁱⁱ	0.93	2.46	3.319 (9)	153
C10—H10...O8 ⁱ	0.93	2.47	3.369 (10)	164
C11—H11...O1 ⁱⁱⁱ	0.93	2.50	3.352 (10)	153
C15—H15...O5	0.93	2.56	2.923 (10)	104
C18—H18...O5 ^{iv}	0.93	2.49	3.409 (11)	168

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y, z+1$; (iii) $x, y, z-1$; (iv) $x, y-1, z$.

Fig. 1

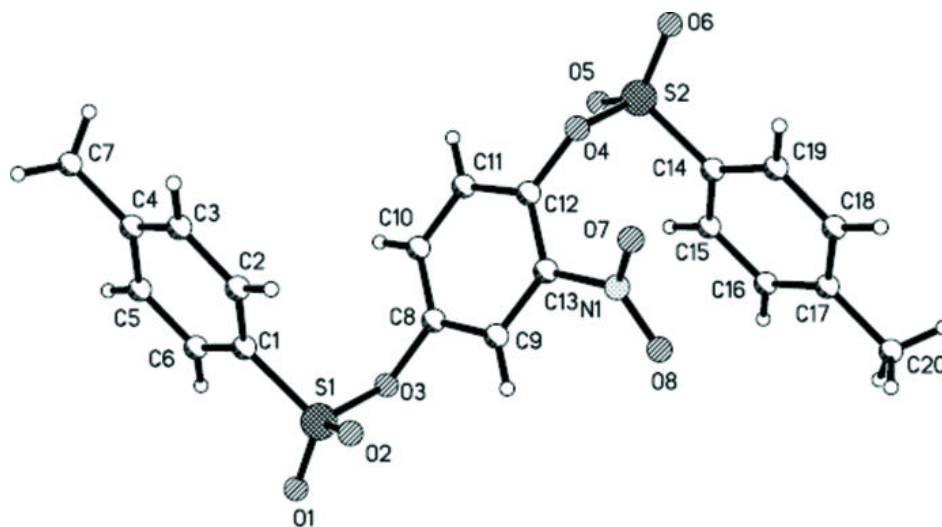


Fig. 2

