Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Nitrophenyl benzenesulfonate

Nagarajan Vembu,[a]* Hazel A. Sparkes[b] and Judith A. K. Howard[b]

[a]Department of Chemistry, Urumu Dhanalakshmi College, Tiruchirappalli 620 019, India, and [b]Durham University, Department of Chemistry, University Science Laboratories, South Road, Durham DH1 3LE, England
Correspondence e-mail: vembu57@yahoo.com

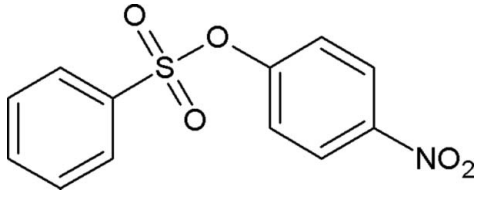
Received 11 July 2007; accepted 13 July 2007

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 16.5.

In the structure of the title compound, $C_{12}H_9NO_5S$, the phenyl and 4-nitrophenyl rings are not coplanar, the dihedral angle being 53.91 (4)°. The structure contains weak intermolecular C—H···O hydrogen bonds and face-to-face π–π interactions between symmetry-related phenyl rings (separation 3.664 Å).

Related literature

For a detailed account of the molecular and supramolecular architectures of aromatic sulfonates, see Manivannan *et al.* (2005) and references cited therein. For related literature, see: Alford *et al.* (1991); Desiraju & Steiner (1999); Jiang *et al.* (1990); Narayanan & Krakow (1983); Spungin *et al.* (1992); Tharakan *et al.* (1992); Yachi *et al.* (1989).



Experimental

Crystal data

$C_{12}H_9NO_5S$
M_r = 279.26
Monoclinic, $P2_1/c$
a = 10.015 (3) Å
b = 10.852 (4) Å
c = 11.396 (4) Å
β = 101.651 (8)°
V = 1213.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 120 (2) K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.799, T_{max} = 1.000 (expected range = 0.755–0.945)
23602 measured reflections
3437 independent reflections
2586 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.093
S = 1.04
3437 reflections
208 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O9^{i}	0.971 (19)	2.567 (19)	3.479 (2)	156.5 (15)
C12—H12···O9^{ii}	0.920 (19)	2.442 (19)	3.188 (2)	138.2 (14)

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

NV thanks the University Grants Commission (UGC), Government of India for a Minor Research Project grant [MRP-2219/06(UGC-SERO)]. JAKH and HAS thank the EPSRC for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2171).

References

Alford, R. L., Honda, S., Lawrence, C. B. & Belmont, J. W. (1991). *Virology*, **183**, 611–619.
Bruker (1998). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 6.45a. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*. New York: Oxford University Press.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Jiang, F. N., Jiang, S., Liu, D., Richter, A. & Levy, J. G. (1990). *J. Immunol. Methods*, **134**, 139–149.
Manivannan, V., Vembu, N., Nallu, M., Sivakumar, K. & Linden, A. (2005). *Acta Cryst.* E**61**, o690–o692.
Narayanan, C. S. & Krakow, J. S. (1983). *Nucleic Acids Res.* **11**, 2701–2716.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1998). *SADABS*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Spungin, B., Levinshal, T., Rubenstein, S. & Breitbart, H. (1992). *FEBS Lett.* **311**, 155–160.
Tharakan, J., Highsmith, F., Clark, D. & Drohsn, W. (1992). *J. Chromatogr.* **595**, 103–111.
Yachi, K., Sugiyama, Y., Sawada, Y., Iga, T., Ikeda, Y., Toda, G. & Hanano, M. (1989). *Biochim. Biophys. Acta*, **978**, 1–7.

supplementary materials

Acta Cryst. (2007). E**63**, o3543 [**doi:10.1107/S1600536807034381**]

4-Nitrophenyl benzenesulfonate

N. Vembu, H. A. Sparkes and J. A. K. Howard

Comment

Aromatic sulfonates are used in monitoring the merging of lipids (Yachi *et al.*, 1989) and in many other fields (Spungin *et al.*, 1992, Tharakan *et al.*,1992, Alford *et al.*, 1991, Jiang *et al.*, 1990, Narayanan & Krakow, 1983). An X-ray study of the title compound was undertaken in order to determine its crystal and molecular structure owing to the biological importance of its analogues. The molecular structure of the title compound, $C_{12}H_9NO_5S$, is shown in Fig. 1 with selected torsion angles provided in Table 1. The S—C, S—O and S=O bond lengths are all comparable to those found in related structures previously reported by our research group (Manivannan *et al.* 2005 & references cited therein).

A Newman projection along the O10—S1 bond is shown in Fig. 2. Using C11 as a reference point, the orientations of the two sulfonyl oxygen atoms (O8 and O9) and the phenyl carbon (C2) have been deduced from the corresponding torsion angles (C11–O10–S1–O8/O9/C2). Helical nomenclature is followed in assigning + or -synclinal and -antiperiplanar conformations. The C2–S1–O10–C11 torsion angle of 75.2 (1)° corresponds to +synclinal conformation. The dihedral angle between the mean planes of the phenyl and 4-nitrophenyl rings of 53.91 (4)° shows that the two rings are not coplanar. This is similar to the situation reported by us for other aromatic sulfonates (Manivannan *et al.* 2005 & references cited therein).

The crystal structure of the title compound is stabilized by the presence of weak intermolecular C—H···O (Fig. 3) (Desiraju *et al.*, 1999) (Table 2) and π···π interactions. The symmetry related phenyl rings (C2—C7) [$2 - x$, $1 - y$, $-z$] interact in a face to face manner with a separation of 3.664 Å.

Experimental

Benzenesulfonyl chloride (10 mmol), dissolved in acetone (10 ml), was added dropwise to 4-nitrophenol (10 mmol) in aqueous NaOH (8 ml, 5%) with constant stirring. The precipitate (6.5 mmol, yield 65%) was filtered and recrystallized from an acetone/ethanol (1:10) mixture.

Refinement

All H atoms were located in difference maps and their positions and isotropic displacement parameters freely refined. The range of refined C—H distances was 0.91 (2) − 0.99 (2) Å.

Figures

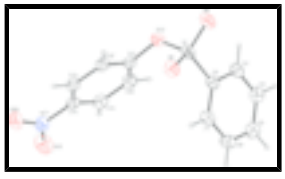


Fig. 1. The molecular structure of the title compound, with the atoms labelled and displacement ellipsoids drawn at the 50% probability level for all non-H atoms. H-atoms are drawn as spheres of arbitrary radius.

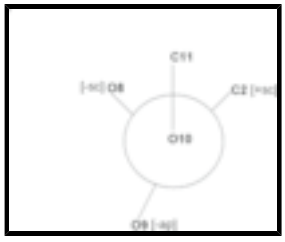


Fig. 2. A Newman projection along the O10—S1 bond with C11 as a reference point, +/-*sc* = +/-synclinal, -*ap* = -antiperiplanar.

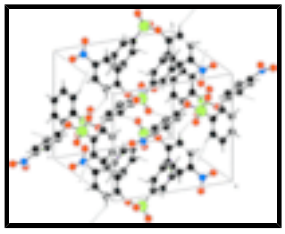


Fig. 3. The molecular packing. Dashed lines represent the weak C—H···O interactions.

4-Nitrophenyl benzenesulfonate

Crystal data

$C_{12}H_9NO_5S$	F_{000} = 576
M_r = 279.26	D_x = 1.529 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 340-342 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.015 (3) Å	Cell parameters from 8716 reflections
b = 10.852 (4) Å	θ = 2.6–30.0º
c = 11.396 (4) Å	μ = 0.28 mm^{-1}
β = 101.651 (8)º	T = 120 (2) K
V = 1213.0 (7) Å^3	Block, colourless
Z = 4	0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer	3437 independent reflections
Radiation source: fine-focus sealed tube	2586 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
Detector resolution: 8 pixels mm^{-1}	θ_{max} = 30.3º
T = 120(2) K	θ_{min} = 2.1º
ω scans	h = −14→13
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)	k = −15→15
T_{min} = 0.799, T_{max} = 1.000	l = −15→15
23602 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	All H-atom parameters refined
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.5272P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3437 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.88009 (4)	0.64514 (3)	0.20115 (3)	0.02644 (10)
C2	0.84763 (14)	0.53463 (13)	0.08707 (13)	0.0241 (3)
C3	0.77611 (15)	0.56938 (15)	−0.02609 (13)	0.0270 (3)
C4	0.75429 (15)	0.48225 (16)	−0.11640 (14)	0.0298 (3)
C5	0.80280 (15)	0.36285 (15)	−0.09411 (14)	0.0302 (3)
C6	0.87286 (16)	0.32943 (15)	0.01874 (15)	0.0312 (3)
C7	0.89596 (15)	0.41514 (14)	0.11100 (14)	0.0278 (3)
O8	0.98137 (11)	0.59973 (11)	0.29756 (9)	0.0316 (2)
O9	0.89369 (13)	0.76432 (10)	0.15216 (10)	0.0361 (3)
O10	0.73797 (11)	0.65581 (10)	0.24513 (9)	0.0296 (2)
C11	0.70056 (15)	0.56091 (13)	0.31653 (13)	0.0248 (3)
C12	0.75723 (16)	0.55939 (14)	0.43750 (13)	0.0270 (3)
C13	0.71255 (15)	0.47233 (14)	0.50931 (13)	0.0273 (3)
C14	0.61342 (14)	0.38957 (13)	0.45633 (13)	0.0250 (3)
C15	0.55842 (15)	0.38921 (15)	0.33496 (14)	0.0278 (3)
C16	0.60276 (15)	0.47702 (15)	0.26344 (13)	0.0285 (3)
N17	0.56559 (13)	0.29760 (13)	0.53293 (12)	0.0313 (3)
O18	0.59839 (14)	0.31087 (12)	0.64123 (11)	0.0432 (3)
O19	0.49469 (14)	0.21269 (13)	0.48477 (12)	0.0470 (3)
H3	0.7429 (19)	0.6529 (17)	−0.0389 (16)	0.034 (5)*
H4	0.7063 (19)	0.5073 (18)	−0.1976 (17)	0.035 (5)*
H5	0.7882 (19)	0.3017 (17)	−0.1583 (16)	0.035 (5)*

H6	0.910 (2)	0.2527 (19)	0.0343 (17)	0.040 (5)*
H7	0.9479 (19)	0.3944 (18)	0.1900 (17)	0.037 (5)*
H12	0.8242 (18)	0.6151 (17)	0.4690 (16)	0.032 (5)*
H13	0.7501 (19)	0.4703 (17)	0.5940 (17)	0.037 (5)*
H15	0.4911 (19)	0.3330 (17)	0.3031 (16)	0.033 (5)*
H16	0.5667 (19)	0.4819 (17)	0.1794 (17)	0.036 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03116 (19)	0.02337 (18)	0.02263 (18)	−0.00350 (14)	0.00035 (13)	0.00245 (14)
C2	0.0232 (6)	0.0247 (7)	0.0236 (7)	−0.0038 (5)	0.0031 (5)	0.0018 (5)
C3	0.0258 (7)	0.0282 (8)	0.0256 (7)	0.0013 (6)	0.0020 (5)	0.0038 (6)
C4	0.0238 (7)	0.0379 (9)	0.0262 (7)	−0.0013 (6)	0.0014 (6)	0.0000 (6)
C5	0.0244 (7)	0.0327 (8)	0.0332 (8)	−0.0067 (6)	0.0053 (6)	−0.0058 (7)
C6	0.0285 (7)	0.0246 (8)	0.0395 (9)	−0.0027 (6)	0.0047 (6)	0.0006 (6)
C7	0.0261 (7)	0.0270 (8)	0.0287 (7)	−0.0019 (6)	0.0015 (6)	0.0054 (6)
O8	0.0310 (6)	0.0351 (6)	0.0252 (5)	−0.0033 (5)	−0.0024 (4)	0.0015 (4)
O9	0.0514 (7)	0.0252 (6)	0.0289 (6)	−0.0094 (5)	0.0014 (5)	0.0040 (4)
O10	0.0357 (6)	0.0248 (5)	0.0275 (5)	0.0053 (4)	0.0044 (4)	0.0047 (4)
C11	0.0287 (7)	0.0218 (7)	0.0239 (7)	0.0052 (5)	0.0052 (5)	0.0003 (5)
C12	0.0315 (7)	0.0238 (7)	0.0243 (7)	−0.0010 (6)	0.0023 (6)	−0.0053 (6)
C13	0.0309 (7)	0.0298 (8)	0.0202 (7)	0.0025 (6)	0.0028 (6)	−0.0033 (6)
C14	0.0251 (7)	0.0245 (7)	0.0263 (7)	0.0052 (5)	0.0073 (5)	−0.0002 (5)
C15	0.0237 (7)	0.0301 (8)	0.0283 (7)	0.0002 (6)	0.0024 (6)	−0.0052 (6)
C16	0.0274 (7)	0.0343 (8)	0.0217 (7)	0.0029 (6)	0.0001 (6)	−0.0024 (6)
N17	0.0275 (6)	0.0331 (7)	0.0346 (7)	0.0027 (5)	0.0093 (5)	0.0035 (6)
O18	0.0566 (8)	0.0446 (7)	0.0301 (6)	−0.0018 (6)	0.0129 (6)	0.0064 (5)
O19	0.0420 (7)	0.0467 (8)	0.0516 (8)	−0.0171 (6)	0.0079 (6)	0.0026 (6)

Geometric parameters (Å, °)

S1—O8	1.4243 (11)	O10—C11	1.4094 (18)
S1—O9	1.4262 (12)	C11—C12	1.381 (2)
S1—O10	1.6057 (12)	C11—C16	1.384 (2)
S1—C2	1.7503 (15)	C12—C13	1.382 (2)
C2—C7	1.392 (2)	C12—H12	0.920 (19)
C2—C3	1.395 (2)	C13—C14	1.384 (2)
C3—C4	1.382 (2)	C13—H13	0.962 (18)
C3—H3	0.967 (19)	C14—C15	1.382 (2)
C4—C5	1.389 (2)	C14—N17	1.469 (2)
C4—H4	0.991 (19)	C15—C16	1.384 (2)
C5—C6	1.383 (2)	C15—H15	0.927 (19)
C5—H5	0.976 (19)	C16—H16	0.954 (19)
C6—C7	1.388 (2)	N17—O18	1.2198 (18)
C6—H6	0.91 (2)	N17—O19	1.2236 (19)
C7—H7	0.971 (19)		
O8—S1—O9	120.42 (7)	C2—C7—H7	119.9 (11)

O8—S1—O10	108.79 (7)	C11—O10—S1	118.90 (9)
O9—S1—O10	102.56 (7)	C12—C11—C16	122.72 (14)
O8—S1—C2	109.42 (7)	C12—C11—O10	118.79 (13)
O9—S1—C2	110.41 (7)	C16—C11—O10	118.39 (13)
O10—S1—C2	103.76 (6)	C11—C12—C13	118.84 (14)
C7—C2—C3	121.77 (14)	C11—C12—H12	120.1 (11)
C7—C2—S1	119.19 (11)	C13—C12—H12	121.0 (11)
C3—C2—S1	119.02 (12)	C12—C13—C14	118.35 (14)
C4—C3—C2	118.55 (14)	C12—C13—H13	120.1 (11)
C4—C3—H3	122.1 (11)	C14—C13—H13	121.6 (11)
C2—C3—H3	119.4 (11)	C15—C14—C13	122.99 (14)
C3—C4—C5	120.34 (15)	C15—C14—N17	118.77 (14)
C3—C4—H4	118.8 (11)	C13—C14—N17	118.24 (13)
C5—C4—H4	120.9 (11)	C14—C15—C16	118.50 (14)
C6—C5—C4	120.51 (15)	C14—C15—H15	120.4 (11)
C6—C5—H5	119.3 (11)	C16—C15—H15	121.1 (11)
C4—C5—H5	120.2 (11)	C11—C16—C15	118.58 (14)
C5—C6—C7	120.28 (15)	C11—C16—H16	119.6 (12)
C5—C6—H6	122.0 (12)	C15—C16—H16	121.8 (12)
C7—C6—H6	117.6 (12)	O18—N17—O19	123.79 (14)
C6—C7—C2	118.55 (14)	O18—N17—C14	117.88 (14)
C6—C7—H7	121.5 (11)	O19—N17—C14	118.33 (13)
O8—S1—C2—C7	13.37 (14)	S1—O10—C11—C12	79.98 (15)
O9—S1—C2—C7	148.12 (12)	S1—O10—C11—C16	−103.52 (14)
O10—S1—C2—C7	−102.61 (12)	C16—C11—C12—C13	−1.5 (2)
O8—S1—C2—C3	−165.46 (11)	O10—C11—C12—C13	174.88 (13)
O9—S1—C2—C3	−30.71 (14)	C11—C12—C13—C14	0.5 (2)
O10—S1—C2—C3	78.56 (12)	C12—C13—C14—C15	0.8 (2)
C7—C2—C3—C4	−0.6 (2)	C12—C13—C14—N17	−179.67 (13)
S1—C2—C3—C4	178.25 (11)	C13—C14—C15—C16	−1.2 (2)
C2—C3—C4—C5	0.1 (2)	N17—C14—C15—C16	179.26 (13)
C3—C4—C5—C6	0.3 (2)	C12—C11—C16—C15	1.0 (2)
C4—C5—C6—C7	−0.2 (2)	O10—C11—C16—C15	−175.31 (13)
C5—C6—C7—C2	−0.2 (2)	C14—C15—C16—C11	0.3 (2)
C3—C2—C7—C6	0.6 (2)	C15—C14—N17—O18	−168.62 (14)
S1—C2—C7—C6	−178.16 (11)	C13—C14—N17—O18	11.8 (2)
O8—S1—O10—C11	−41.26 (12)	C15—C14—N17—O19	10.9 (2)
O9—S1—O10—C11	−169.86 (10)	C13—C14—N17—O19	−168.63 (14)
C2—S1—O10—C11	75.15 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O8	0.971 (19)	2.533 (19)	2.921 (2)	103.8 (13)
C7—H7···O9^{i}	0.971 (19)	2.567 (19)	3.479 (2)	156.5 (15)
C12—H12···O9^{ii}	0.920 (19)	2.442 (19)	3.188 (2)	138.2 (14)

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

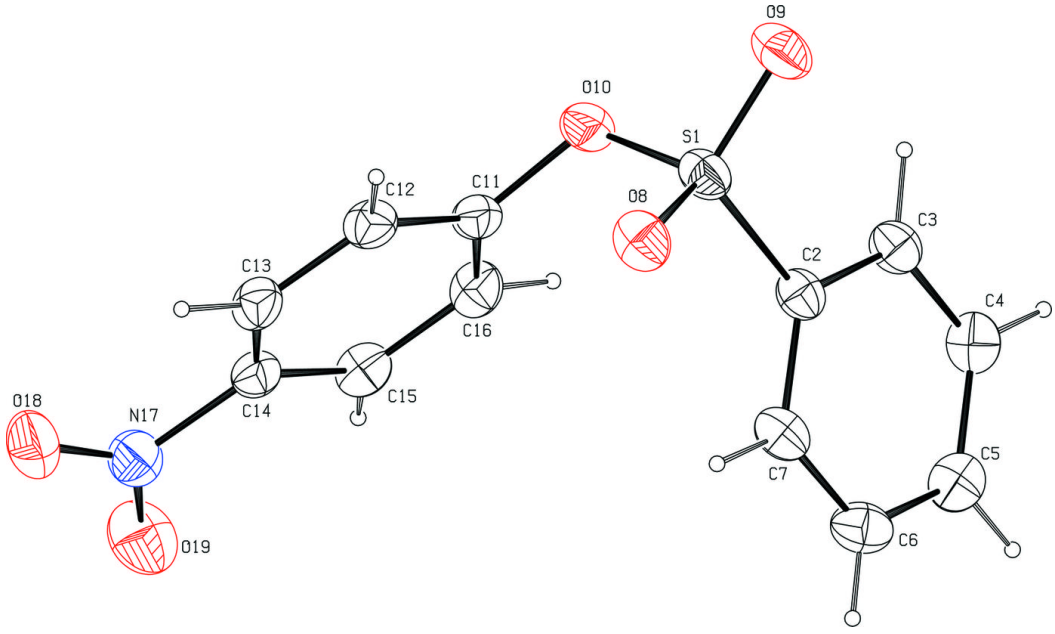


Fig. 2

,

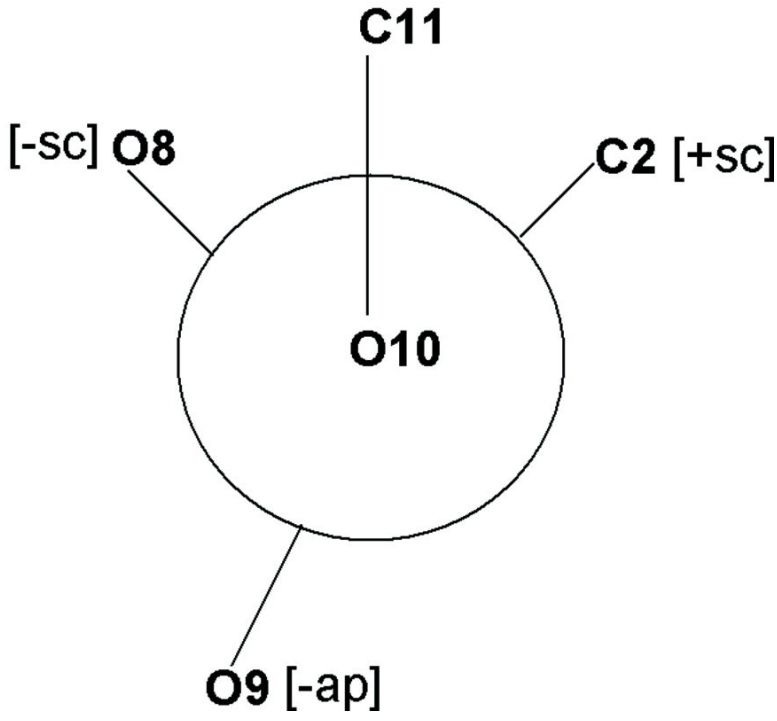


Fig. 3