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2-Naphthyl benzenesulfonate

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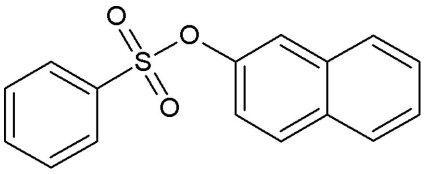
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.127; data-to-parameter ratio = 17.1.

The phenyl and naphthyl ring systems are at an angle of 47.57 (9)° in the title compound, $C_{16}H_{12}O_3S$. Only weak C—H···O interactions are present in the crystal structure.

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

$C_{16}H_{12}O_3S$
M_r = 284.32
Orthorhombic, *Pbcn*
a = 11.8910 (11) Å
b = 10.8909 (12) Å
c = 20.958 (2) Å
V = 2714.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 120 (2) K
0.24 × 0.16 × 0.08 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{\min}$ = 0.814, $T_{\max}$ = 1.000 (expected range = 0.922–0.951)
19056 measured reflections
3917 independent reflections
2262 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.127
S = 1.00
3917 reflections
229 parameters
All H-atom parameters refined
$\Delta\rho_{\max}$ = 0.33 e Å^{-3}
$\Delta\rho_{\min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O9$^{\rm i}$	0.93 (2)	2.55 (2)	3.448 (3)	161.6 (19)
C13—H13···O8$^{\rm ii}$	0.99 (2)	2.52 (2)	3.432 (3)	152.1 (18)
C18—H18···O9$^{\rm iii}$	0.98 (2)	2.53 (2)	3.457 (3)	157.8 (17)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2026).

References

Alford, R. L., Honda, S., Lawrence, C. B. & Belmont, J. W. (1991). *Virology*, **183**, 611–619.
Bruker (1998). *SMART* (Version 5.054) and *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

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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 (I) was undertaken in order to determine its crystal and molecular structure owing to the biological importance of its analogues. The molecular structure of (I) is shown in Fig. 1 with selected geometric parameters provided in Table 1. The S—C, S—O and S=O bond lengths are comparable with 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 provided 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 nomeclature is employed to assign + or -synclinal and +antiperiplanar conformations. The C2–S1–O10–C11 torsion angle of 60.6 (2)° corresponds to +synclinal conformation; as expected the dihedral angle between the mean planes of the phenyl and naphthyl rings of 47.57 (7)° 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 (I) is stabilized by weak intermolecular C—H···O interactions (Desiraju *et al.*, 1999) (Table 2, Fig. 3).

Experimental

Benzenesulfonyl chloride (10 mmol), dissolved in acetone, was added dropwise to 2-naphthol (10 mmol) in aqueous NaOH (8 ml, 5%) with constant stirring. The precipitate (6.5 mmol, yield 65%) was filtered and recrystallized from aqueous ethanol.

Refinement

All H-atoms were located in difference maps and their positions and isotropic displacement parameters freely refined.

Figures

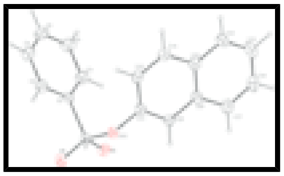

Fig. 1. The asymmetric unit of (I) with the atoms labelled and displacement ellipsoids depicted at the 50% probability level for all non-H atoms. H-atoms are drawn as spheres of arbitrary radius

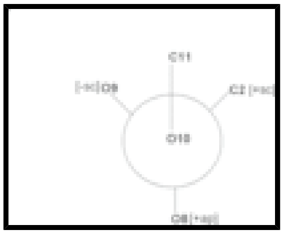

Fig. 2. A Newman projection along the O10—S1 bond with C11 as a reference point, +/-*sc* = +/-synclinal, -*ap* = -antiperiplanar.

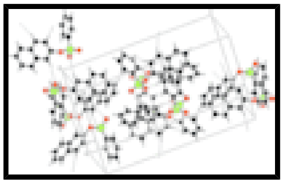

Fig. 3. The molecular packing viewed down the *b*-axis. Dashed lines represent the weak C—H···O interactions within the lattice.

2-Napthyl benzenesulfonate

Crystal data

$C_{16}H_{12}O_3S$

$M_r = 284.32$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 11.8910\ (11)$ Å

$b = 10.8909\ (12)$ Å

$c = 20.958\ (2)$ Å

$V = 2714.1\ (5)$ Å^3

$Z = 8$

$F_{000} = 1184$

$D_x = 1.392$ Mg m^{-3}

Melting point: 394-396 K

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 2747 reflections

θ = 2.5–27.3°

$\mu = 0.24$ mm^{-1}

$T = 120\ (2)$ K

Plate, colourless

0.24 × 0.16 × 0.08 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8 pixels mm^{-1}

$T = 120(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1998a)

$T_{\min} = 0.814$, $T_{\max} = 1.000$

19056 measured reflections

3917 independent reflections

2262 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.089$

$\theta_{\max} = 30.4°$

$\theta_{\min} = 1.9°$

$h = -16\rightarrow16$

$k = -15\rightarrow14$

$l = -29\rightarrow21$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.047$	All H-atom parameters refined
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.8434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3917 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
229 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.15762 (4)	0.88595 (5)	0.40500 (2)	0.01934 (14)
C2	0.30301 (18)	0.8898 (2)	0.39181 (10)	0.0187 (4)
C3	0.3510 (2)	0.8047 (2)	0.35098 (11)	0.0250 (5)
C4	0.4658 (2)	0.8075 (2)	0.34121 (12)	0.0315 (6)
C5	0.5312 (2)	0.8953 (2)	0.37184 (12)	0.0313 (6)
C6	0.4828 (2)	0.9788 (2)	0.41258 (13)	0.0308 (6)
C7	0.36756 (19)	0.9777 (2)	0.42299 (11)	0.0248 (5)
O8	0.10154 (13)	0.83470 (15)	0.35111 (7)	0.0274 (4)
O9	0.12184 (13)	1.00159 (14)	0.42973 (7)	0.0255 (4)
O10	0.14112 (12)	0.78362 (13)	0.45886 (7)	0.0206 (3)
C11	0.19407 (19)	0.8014 (2)	0.51926 (10)	0.0188 (5)
C12	0.29256 (19)	0.7343 (2)	0.53019 (11)	0.0216 (5)
C13	0.3430 (2)	0.7432 (2)	0.58838 (11)	0.0227 (5)
C14	0.3508 (2)	0.8323 (2)	0.69741 (11)	0.0261 (5)
C15	0.3072 (2)	0.9087 (2)	0.74265 (12)	0.0311 (6)
C16	0.2074 (2)	0.9743 (2)	0.73036 (12)	0.0319 (6)
C17	0.1535 (2)	0.9632 (2)	0.67294 (11)	0.0270 (5)
C18	0.14591 (19)	0.8753 (2)	0.56366 (10)	0.0200 (5)
C19	0.29784 (19)	0.8194 (2)	0.63705 (11)	0.0207 (5)
C20	0.19838 (19)	0.8870 (2)	0.62448 (10)	0.0201 (5)
H3	0.306 (2)	0.745 (2)	0.3302 (11)	0.024 (6)*
H4	0.503 (2)	0.749 (2)	0.3146 (11)	0.030 (7)*

H5	0.610 (2)	0.894 (2)	0.3643 (11)	0.028 (6)*
H6	0.523 (2)	1.039 (2)	0.4320 (12)	0.041 (8)*
H7	0.3328 (19)	1.037 (2)	0.4526 (12)	0.030 (7)*
H12	0.3242 (19)	0.686 (2)	0.4979 (11)	0.020 (6)*
H13	0.412 (2)	0.695 (2)	0.5964 (11)	0.025 (6)*
H14	0.420 (2)	0.787 (2)	0.7050 (11)	0.030 (7)*
H15	0.343 (2)	0.916 (2)	0.7828 (13)	0.038 (7)*
H16	0.182 (2)	1.024 (3)	0.7619 (15)	0.051 (9)*
H17	0.081 (2)	1.005 (2)	0.6640 (10)	0.022 (6)*
H18	0.076 (2)	0.918 (2)	0.5537 (10)	0.019 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0171 (2)	0.0239 (3)	0.0170 (3)	−0.0006 (2)	−0.0006 (2)	0.0004 (2)
C2	0.0173 (10)	0.0218 (11)	0.0172 (10)	−0.0002 (9)	−0.0022 (8)	0.0032 (9)
C3	0.0253 (12)	0.0258 (13)	0.0241 (12)	0.0005 (11)	−0.0020 (10)	−0.0049 (9)
C4	0.0284 (13)	0.0372 (15)	0.0289 (13)	0.0110 (12)	0.0037 (11)	−0.0033 (11)
C5	0.0182 (11)	0.0428 (16)	0.0328 (14)	0.0026 (12)	0.0033 (11)	0.0128 (12)
C6	0.0238 (13)	0.0322 (14)	0.0365 (15)	−0.0080 (11)	−0.0007 (11)	0.0025 (12)
C7	0.0243 (12)	0.0227 (12)	0.0273 (12)	−0.0032 (10)	0.0030 (10)	−0.0013 (10)
O8	0.0240 (9)	0.0384 (10)	0.0199 (8)	−0.0049 (7)	−0.0037 (7)	−0.0012 (7)
O9	0.0245 (8)	0.0258 (9)	0.0262 (9)	0.0065 (7)	0.0022 (7)	0.0005 (7)
O10	0.0212 (8)	0.0238 (8)	0.0168 (7)	−0.0054 (6)	−0.0014 (6)	−0.0001 (6)
C11	0.0209 (10)	0.0197 (11)	0.0160 (10)	−0.0034 (9)	−0.0012 (9)	0.0012 (9)
C12	0.0242 (12)	0.0196 (11)	0.0211 (11)	0.0009 (9)	0.0033 (10)	−0.0004 (9)
C13	0.0202 (11)	0.0229 (11)	0.0248 (12)	0.0004 (10)	0.0008 (10)	0.0006 (9)
C14	0.0270 (12)	0.0286 (13)	0.0227 (12)	−0.0019 (11)	−0.0055 (11)	0.0040 (10)
C15	0.0410 (15)	0.0333 (14)	0.0191 (12)	−0.0080 (12)	−0.0065 (11)	0.0027 (10)
C16	0.0455 (16)	0.0301 (14)	0.0201 (12)	0.0013 (12)	0.0050 (12)	−0.0039 (11)
C17	0.0318 (13)	0.0277 (13)	0.0216 (12)	0.0044 (11)	0.0046 (11)	0.0014 (10)
C18	0.0183 (11)	0.0227 (11)	0.0188 (11)	0.0000 (10)	−0.0005 (9)	0.0038 (9)
C19	0.0215 (11)	0.0198 (11)	0.0210 (11)	−0.0038 (9)	−0.0004 (9)	0.0029 (9)
C20	0.0248 (11)	0.0178 (11)	0.0177 (10)	−0.0018 (10)	0.0005 (9)	0.0036 (9)

Geometric parameters (Å, °)

S1—O8	1.4254 (16)	C11—C12	1.399 (3)
S1—O9	1.4267 (16)	C12—C13	1.363 (3)
S1—O10	1.5983 (15)	C12—H12	0.93 (2)
S1—C2	1.751 (2)	C13—C19	1.420 (3)
C2—C3	1.384 (3)	C13—H13	0.99 (2)
C2—C7	1.390 (3)	C14—C15	1.363 (4)
C3—C4	1.382 (3)	C14—C19	1.420 (3)
C3—H3	0.94 (2)	C14—H14	0.97 (3)
C4—C5	1.389 (4)	C15—C16	1.409 (4)
C4—H4	0.95 (2)	C15—H15	0.95 (3)
C5—C6	1.374 (4)	C16—C17	1.368 (3)
C5—H5	0.95 (3)	C16—H16	0.91 (3)

C6—C7	1.388 (3)	C17—C20	1.416 (3)
C6—H6	0.91 (3)	C17—H17	0.99 (2)
C7—H7	0.99 (2)	C18—C20	1.425 (3)
O10—C11	1.427 (2)	C18—H18	0.98 (2)
C11—C18	1.358 (3)	C19—C20	1.418 (3)

O8—S1—O9	119.60 (10)	C13—C12—C11	118.5 (2)
O8—S1—O10	103.24 (9)	C13—C12—H12	120.8 (14)
O9—S1—O10	108.81 (9)	C11—C12—H12	120.7 (14)
O8—S1—C2	110.25 (10)	C12—C13—C19	121.2 (2)
O9—S1—C2	109.31 (10)	C12—C13—H13	118.7 (13)
O10—S1—C2	104.43 (9)	C19—C13—H13	120.1 (13)
C3—C2—C7	121.6 (2)	C15—C14—C19	120.8 (2)
C3—C2—S1	119.23 (18)	C15—C14—H14	121.2 (14)
C7—C2—S1	119.16 (17)	C19—C14—H14	118.0 (14)
C4—C3—C2	119.0 (2)	C14—C15—C16	120.1 (2)
C4—C3—H3	120.2 (14)	C14—C15—H15	119.8 (16)
C2—C3—H3	120.8 (15)	C16—C15—H15	120.0 (16)
C3—C4—C5	120.0 (2)	C17—C16—C15	120.7 (2)
C3—C4—H4	121.9 (15)	C17—C16—H16	122.7 (19)
C5—C4—H4	118.1 (15)	C15—C16—H16	116.6 (19)
C6—C5—C4	120.6 (2)	C16—C17—C20	120.4 (2)
C6—C5—H5	121.7 (15)	C16—C17—H17	122.1 (13)
C4—C5—H5	117.7 (14)	C20—C17—H17	117.4 (13)
C5—C6—C7	120.3 (2)	C11—C18—C20	118.8 (2)
C5—C6—H6	122.2 (17)	C11—C18—H18	119.8 (13)
C7—C6—H6	117.4 (17)	C20—C18—H18	121.5 (13)
C6—C7—C2	118.5 (2)	C20—C19—C14	119.0 (2)
C6—C7—H7	120.4 (14)	C20—C19—C13	119.0 (2)
C2—C7—H7	121.0 (14)	C14—C19—C13	122.0 (2)
C11—O10—S1	118.55 (13)	C17—C20—C19	119.0 (2)
C18—C11—C12	123.4 (2)	C17—C20—C18	122.0 (2)
C18—C11—O10	120.15 (19)	C19—C20—C18	119.0 (2)
C12—C11—O10	116.35 (19)		

O8—S1—C2—C3	−27.2 (2)	O10—C11—C12—C13	−176.67 (19)
O9—S1—C2—C3	−160.58 (17)	C11—C12—C13—C19	−0.5 (3)
O10—S1—C2—C3	83.12 (19)	C19—C14—C15—C16	1.2 (4)
O8—S1—C2—C7	153.28 (17)	C14—C15—C16—C17	−0.6 (4)
O9—S1—C2—C7	19.9 (2)	C15—C16—C17—C20	−1.0 (4)
O10—S1—C2—C7	−96.41 (19)	C12—C11—C18—C20	0.7 (3)
C7—C2—C3—C4	0.1 (4)	O10—C11—C18—C20	177.35 (18)
S1—C2—C3—C4	−179.43 (19)	C15—C14—C19—C20	−0.2 (3)
C2—C3—C4—C5	−0.4 (4)	C15—C14—C19—C13	178.2 (2)
C3—C4—C5—C6	0.8 (4)	C12—C13—C19—C20	0.0 (3)
C4—C5—C6—C7	−0.9 (4)	C12—C13—C19—C14	−178.4 (2)
C5—C6—C7—C2	0.5 (4)	C16—C17—C20—C19	2.0 (3)
C3—C2—C7—C6	−0.2 (3)	C16—C17—C20—C18	−178.6 (2)
S1—C2—C7—C6	179.36 (18)	C14—C19—C20—C17	−1.4 (3)
O8—S1—O10—C11	175.90 (15)	C13—C19—C20—C17	−179.8 (2)

O9—S1—O10—C11	−56.06 (17)	C14—C19—C20—C18	179.2 (2)
C2—S1—O10—C11	60.58 (17)	C13—C19—C20—C18	0.8 (3)
S1—O10—C11—C18	81.0 (2)	C11—C18—C20—C17	179.5 (2)
S1—O10—C11—C12	−102.1 (2)	C11—C18—C20—C19	−1.1 (3)
C18—C11—C12—C13	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O9	0.99 (2)	2.58 (2)	2.937 (3)	101.1 (16)
C12—H12···O9^{i}	0.93 (2)	2.55 (2)	3.448 (3)	161.6 (19)
C13—H13···O8^{ii}	0.99 (2)	2.52 (2)	3.432 (3)	152.1 (18)
C18—H18···O9^{iii}	0.98 (2)	2.53 (2)	3.457 (3)	157.8 (17)
C5—H5···Cg2^{iv}	0.95 (3)	3.007	3.554	118.05
C5—H5···Cg3^{v}	0.95 (3)	2.977	3.617	125.99
C6—H6···Cg2^{v}	0.91 (3)	3.209	3.973	142.81
C15—H15···Cg1^{vi}	0.95 (3)	3.073	3.862	141.70

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

Fig. 1

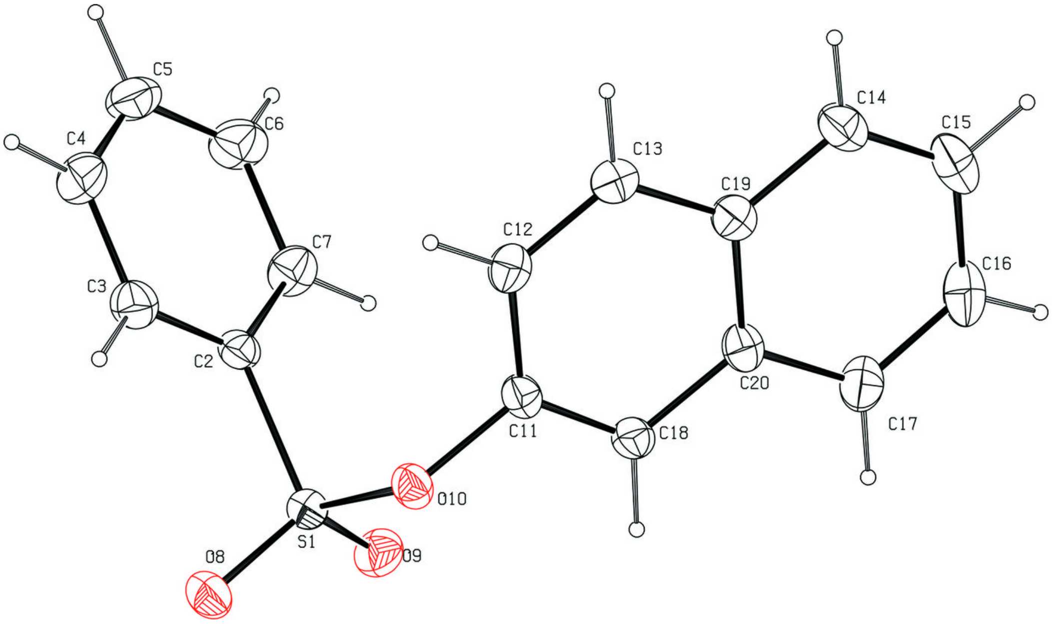
C5
C4
C6
C7
C3
C2
C12
C13
C19
C14
C15
C16
C20
C17
C11
C18
O10
S1
O8
O9

Fig. 2

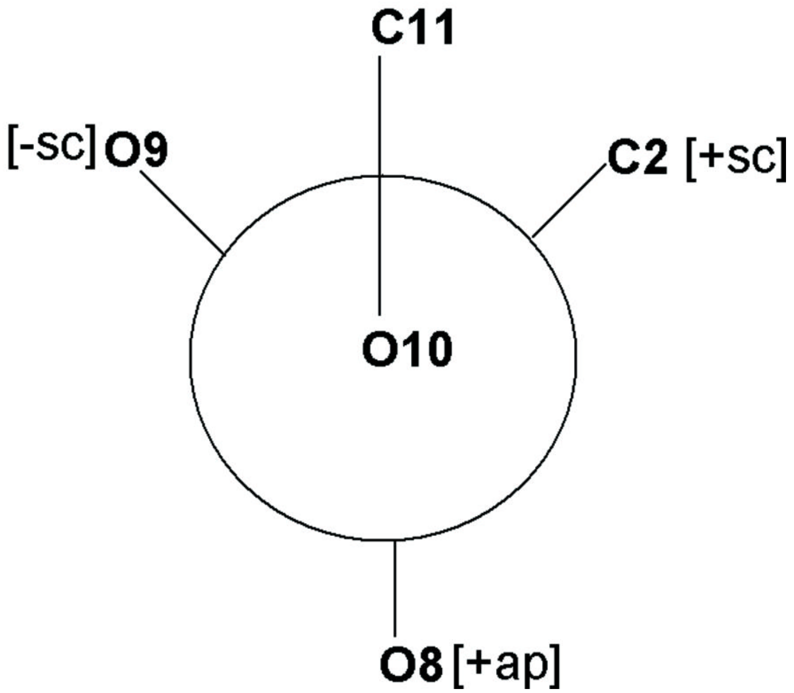

Fig. 3