Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Phenyl naphthalene-2-sulfonate

Jasmine P. Vennila,[a] Helen P. Kavitha,[b] D. John Thiruvadigal[c] and V. Manivannan[d]*

[a]Department of Physics, Panimalar Institute of Technology, Chennai 600 095, India, [b]Department of Chemistry, SRM University, Ramapuram, Chennai 600 089, India, [c]Department of Physics, SRM University, Kattankulathur Campus, Chennai 603 203, India, and [d]Department of Physics, Presidency College, Chennai 600 005, India
Correspondence e-mail: manivan_1999@yahoo.com

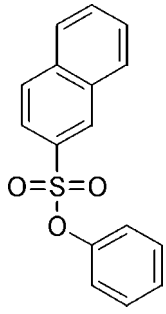
Received 24 October 2008; accepted 31 October 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.106; data-to-parameter ratio = 28.1.

In the crystal structure of the title compound, $C_{16}H_{12}O_3S$, the dihedral angle between the naphthalene ring system and the phenyl ring is 65.21 (3)°. The molecules are linked by intermolecular C—H···O hydrogen bonds, forming a chain along the a axis. The chains are connected through weak C—H···π interactions.

Related literature

For general background, see: Spungin *et al.* (1984); Yachi *et al.* (1989). For related structures, see: Manivannan *et al.* (2005); Ramachandran *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{12}O_3S$
M_r = 284.32
Orthorhombic, $P2_12_12_1$
a = 6.1525 (2) Å
b = 12.7466 (7) Å
c = 17.3414 (10) Å
V = 1359.97 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
0.25 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.942, T_{max} = 0.962
11868 measured reflections
5093 independent reflections
3412 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
S = 1.01
5093 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 1993 Friedel pairs
Flack parameter: −0.03 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2^{i}	0.93	2.51	3.424 (2)	169
C5—H5···$Cg2^{ii}$	0.93	2.96	3.486 (2)	117
C6—H6···$Cg3^{ii}$	0.93	2.94	3.535 (2)	123
C12—H12···$Cg1^{iii}$	0.93	2.94	3.788 (3)	152

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+\frac{3}{2}, -y+2, z+\frac{1}{2}$; (iii) $-x, y+\frac{5}{2}, -z+\frac{1}{2}$. $Cg1$ is the centroid of the C1–C6 ring, $Cg2$ is the centroid of the C7–C9/C14–C16 ring and $Cg3$ is the centroid of the C9–C14 ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2352).

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supporting information

Acta Cryst. (2008). E**64**, o2304 [doi:10.1107/S1600536808035824]

Phenyl naphthalene-2-sulfonate

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S1. Comment

Several compounds containing the *para* -toluene sulfonate moiety are used in the fields of biology and industry. The merging of lipids can be monitored using a derivative of *para*-toluene sulfonate (Yachi *et al.*, 1989). This method has been used in studying the membrane fusion during the acrosome reaction (Spungin *et al.*, 1984).

The geometric parameters in the title compound (I) agree well with the reported values of similar structures (Manivannan *et al.*, 2005; Ramachandran *et al.*, 2007). The phenyl ring makes a dihedral angle of 65.21 (3)° with the naphthalene ring system. The torsion angles of O2—S1—C7—C8 and O3—S1—C7—C16 [2.04 (15)° and 46.94 (15)°, respectively] indicate the *syn* conformation of the sulfonyl moiety. The crystal structure is stabilized through weak intermolecular C—H···O and C—H···π interactions (Fig. 2 and Table 1). Cg1, Cg2 and Cg3 are the centroids of the C1–C6 ring, the C7–C9/C14–C16 ring and the C9–C14 ring, respectively.

S2. Experimental

2-Naphthalene sulfonyl chloride (2.5 mmol) dissolved in acetone (4 ml) was added dropwise to phenol (2.5 mmol) in aqueous NaOH solution (4 ml, 5%) with constant shaking. The precipitated compound (2 mmol, yield 77%) recrystallized from ethanol yielded colourless crystals.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

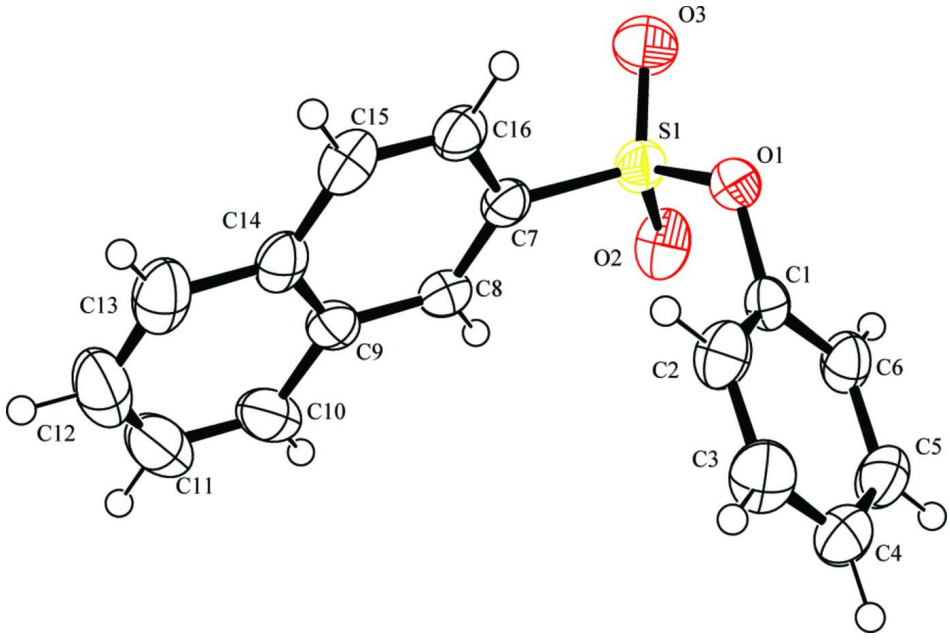

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

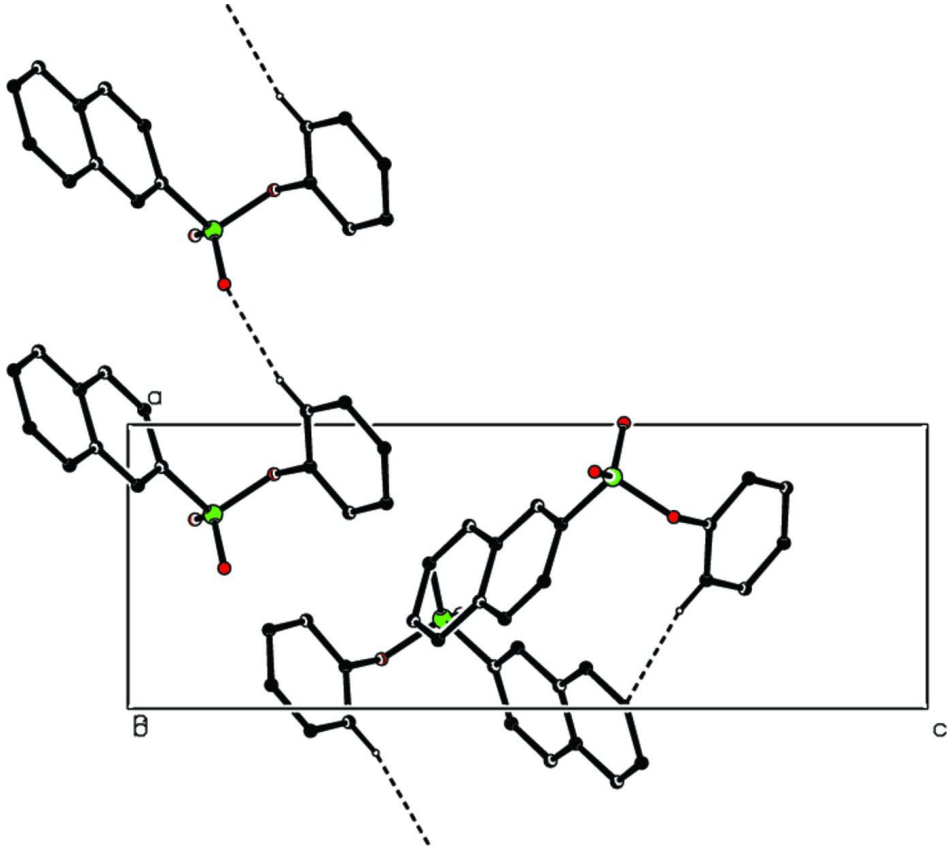

Figure 2

The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for the sake of clarity.

Phenyl naphthalene-2-sulfonate

Crystal data

$C_{16}H_{12}O_3S$
$M_r = 284.32$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.1525$ (2) Å
$b = 12.7466$ (7) Å
$c = 17.3414$ (10) Å
$V = 1359.97$ (12) Å^3
$Z = 4$
$F(000) = 592$
$D_x = 1.389$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4818 reflections
$\theta = 2.2$–$25.4°$
$\mu = 0.24$ mm^{-1}
$T = 295$ K
Tablet, colourless
0.25 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.942$, $T_{max} = 0.962$
11868 measured reflections
5093 independent reflections
3412 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 34.9°$, $\theta_{min} = 2.4°$
$h = -9 \rightarrow 5$
$k = -19 \rightarrow 18$
$l = -25 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.106$
$S = 1.01$
5093 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.0596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack (1983), 1993 Friedel pairs
Absolute structure parameter: −0.03 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.68361 (7)	0.89579 (3)	0.10630 (3)	0.03997 (11)
O1	0.8255 (2)	0.88973 (9)	0.18279 (6)	0.0403 (3)
O2	0.4945 (2)	0.95689 (12)	0.12058 (8)	0.0527 (4)
O3	0.6661 (3)	0.78918 (10)	0.08397 (9)	0.0646 (4)
C1	0.8523 (3)	0.98154 (12)	0.22766 (9)	0.0332 (3)
C2	1.0472 (3)	1.03331 (16)	0.22378 (11)	0.0438 (4)
H2	1.1557	1.0114	0.1901	0.053*
C3	1.0781 (3)	1.11934 (17)	0.27152 (13)	0.0537 (5)
H3	1.2089	1.1558	0.2701	0.064*
C4	0.9168 (3)	1.15065 (16)	0.32060 (12)	0.0513 (5)
H4	0.9389	1.2084	0.3524	0.062*
C5	0.7234 (3)	1.09789 (16)	0.32342 (10)	0.0497 (5)

H5	0.6144	1.1203	0.3567	0.060*
C6	0.6895 (3)	1.01146 (14)	0.27702 (10)	0.0422 (4)
H6	0.5594	0.9744	0.2792	0.051*
C7	0.8516 (3)	0.96307 (12)	0.04171 (9)	0.0334 (3)
C8	0.7855 (3)	1.05729 (12)	0.01241 (9)	0.0355 (4)
H8	0.6522	1.0855	0.0269	0.043*
C9	0.9203 (3)	1.11168 (13)	−0.03991 (10)	0.0380 (4)
C10	0.8568 (4)	1.20865 (14)	−0.07297 (12)	0.0522 (5)
H10	0.7231	1.2379	−0.0601	0.063*
C11	0.9892 (5)	1.25888 (17)	−0.12299 (12)	0.0652 (6)
H11	0.9458	1.3223	−0.1446	0.078*
C12	1.1911 (5)	1.2161 (2)	−0.14254 (12)	0.0709 (7)
H12	1.2808	1.2516	−0.1769	0.085*
C13	1.2580 (3)	1.12340 (18)	−0.11191 (12)	0.0569 (5)
H13	1.3933	1.0963	−0.1251	0.068*
C14	1.1230 (3)	1.06801 (14)	−0.06014 (10)	0.0405 (4)
C15	1.1837 (3)	0.96940 (15)	−0.02884 (10)	0.0439 (4)
H15	1.3164	0.9399	−0.0425	0.053*
C16	1.0520 (3)	0.91760 (13)	0.02050 (10)	0.0395 (4)
H16	1.0929	0.8527	0.0403	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0443 (2)	0.0406 (2)	0.0350 (2)	−0.00821 (18)	0.00007 (19)	−0.00279 (17)
O1	0.0525 (7)	0.0344 (5)	0.0339 (6)	0.0047 (6)	−0.0012 (5)	0.0021 (5)
O2	0.0361 (7)	0.0768 (9)	0.0451 (8)	−0.0027 (6)	0.0010 (6)	0.0017 (7)
O3	0.0897 (11)	0.0457 (7)	0.0584 (9)	−0.0245 (7)	0.0029 (9)	−0.0083 (6)
C1	0.0381 (10)	0.0353 (7)	0.0262 (7)	0.0012 (6)	−0.0017 (6)	0.0046 (6)
C2	0.0352 (10)	0.0579 (11)	0.0382 (9)	0.0016 (8)	0.0018 (7)	−0.0005 (8)
C3	0.0463 (12)	0.0649 (13)	0.0498 (12)	−0.0151 (10)	−0.0042 (9)	−0.0019 (10)
C4	0.0665 (14)	0.0508 (11)	0.0365 (11)	−0.0090 (9)	−0.0024 (9)	−0.0056 (8)
C5	0.0563 (13)	0.0562 (11)	0.0366 (9)	−0.0022 (9)	0.0132 (8)	−0.0060 (9)
C6	0.0413 (10)	0.0503 (9)	0.0348 (8)	−0.0094 (8)	0.0053 (8)	0.0016 (7)
C7	0.0373 (9)	0.0340 (7)	0.0290 (7)	−0.0004 (6)	−0.0011 (6)	−0.0049 (6)
C8	0.0374 (9)	0.0343 (7)	0.0348 (8)	0.0011 (7)	−0.0017 (7)	−0.0063 (6)
C9	0.0478 (10)	0.0338 (8)	0.0325 (8)	−0.0053 (7)	−0.0064 (7)	−0.0034 (7)
C10	0.0675 (14)	0.0375 (9)	0.0516 (11)	−0.0044 (8)	−0.0138 (10)	0.0012 (8)
C11	0.0953 (18)	0.0482 (11)	0.0521 (14)	−0.0225 (12)	−0.0208 (13)	0.0102 (9)
C12	0.0927 (18)	0.0760 (15)	0.0440 (12)	−0.0440 (15)	−0.0050 (13)	0.0084 (11)
C13	0.0562 (12)	0.0748 (13)	0.0396 (10)	−0.0233 (10)	0.0020 (8)	−0.0062 (10)
C14	0.0419 (11)	0.0515 (10)	0.0280 (8)	−0.0102 (8)	−0.0035 (7)	−0.0074 (7)
C15	0.0378 (10)	0.0594 (10)	0.0347 (9)	0.0062 (9)	−0.0008 (8)	−0.0070 (8)
C16	0.0451 (10)	0.0425 (9)	0.0310 (9)	0.0101 (7)	−0.0023 (7)	−0.0024 (7)

Geometric parameters (Å, º)

S1—O3	1.4172 (13)	C7—C16	1.411 (2)
S1—O2	1.4217 (15)	C8—C9	1.411 (2)
S1—O1	1.5899 (13)	C8—H8	0.9300
S1—C7	1.7487 (17)	C9—C14	1.410 (3)
O1—C1	1.4149 (19)	C9—C10	1.417 (2)
C1—C2	1.370 (2)	C10—C11	1.351 (3)
C1—C6	1.372 (2)	C10—H10	0.9300
C2—C3	1.387 (3)	C11—C12	1.398 (4)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.367 (3)	C12—C13	1.360 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.368 (3)	C13—C14	1.412 (3)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.380 (3)	C14—C15	1.419 (3)
C5—H5	0.9300	C15—C16	1.351 (3)
C6—H6	0.9300	C15—H15	0.9300
C7—C8	1.366 (2)	C16—H16	0.9300
O3—S1—O2	120.72 (10)	C7—C8—C9	119.74 (16)
O3—S1—O1	102.89 (9)	C7—C8—H8	120.1
O2—S1—O1	109.31 (7)	C9—C8—H8	120.1
O3—S1—C7	109.88 (9)	C14—C9—C8	119.07 (16)
O2—S1—C7	109.05 (8)	C14—C9—C10	119.18 (18)
O1—S1—C7	103.52 (7)	C8—C9—C10	121.74 (17)
C1—O1—S1	118.86 (10)	C11—C10—C9	120.4 (2)
C2—C1—C6	122.41 (16)	C11—C10—H10	119.8
C2—C1—O1	118.25 (15)	C9—C10—H10	119.8
C6—C1—O1	119.20 (15)	C10—C11—C12	120.4 (2)
C1—C2—C3	118.10 (17)	C10—C11—H11	119.8
C1—C2—H2	121.0	C12—C11—H11	119.8
C3—C2—H2	121.0	C13—C12—C11	120.9 (2)
C4—C3—C2	120.22 (18)	C13—C12—H12	119.6
C4—C3—H3	119.9	C11—C12—H12	119.6
C2—C3—H3	119.9	C12—C13—C14	120.3 (2)
C3—C4—C5	120.68 (18)	C12—C13—H13	119.8
C3—C4—H4	119.7	C14—C13—H13	119.8
C5—C4—H4	119.7	C9—C14—C13	118.75 (19)
C4—C5—C6	120.22 (17)	C9—C14—C15	119.15 (17)
C4—C5—H5	119.9	C13—C14—C15	122.09 (19)
C6—C5—H5	119.9	C16—C15—C14	121.17 (18)
C1—C6—C5	118.37 (17)	C16—C15—H15	119.4
C1—C6—H6	120.8	C14—C15—H15	119.4
C5—C6—H6	120.8	C15—C16—C7	119.23 (16)
C8—C7—C16	121.62 (16)	C15—C16—H16	120.4
C8—C7—S1	119.58 (13)	C7—C16—H16	120.4
C16—C7—S1	118.80 (12)		

O3—S1—O1—C1	−171.58 (12)	S1—C7—C8—C9	−179.81 (12)
O2—S1—O1—C1	−42.13 (14)	C7—C8—C9—C14	−0.9 (2)
C7—S1—O1—C1	73.97 (13)	C7—C8—C9—C10	178.76 (16)
S1—O1—C1—C2	−104.08 (16)	C14—C9—C10—C11	−0.3 (3)
S1—O1—C1—C6	80.26 (17)	C8—C9—C10—C11	−179.92 (18)
C6—C1—C2—C3	−0.4 (3)	C9—C10—C11—C12	−0.3 (3)
O1—C1—C2—C3	−175.92 (16)	C10—C11—C12—C13	0.2 (3)
C1—C2—C3—C4	−0.1 (3)	C11—C12—C13—C14	0.6 (3)
C2—C3—C4—C5	0.0 (3)	C8—C9—C14—C13	−179.35 (16)
C3—C4—C5—C6	0.6 (3)	C10—C9—C14—C13	1.0 (2)
C2—C1—C6—C5	1.0 (3)	C8—C9—C14—C15	1.5 (2)
O1—C1—C6—C5	176.47 (15)	C10—C9—C14—C15	−178.11 (16)
C4—C5—C6—C1	−1.1 (3)	C12—C13—C14—C9	−1.2 (3)
O3—S1—C7—C8	132.35 (14)	C12—C13—C14—C15	177.93 (18)
O2—S1—C7—C8	−2.04 (15)	C9—C14—C15—C16	−0.8 (3)
O1—S1—C7—C8	−118.32 (13)	C13—C14—C15—C16	−179.89 (18)
O3—S1—C7—C16	−46.94 (15)	C14—C15—C16—C7	−0.6 (3)
O2—S1—C7—C16	178.67 (12)	C8—C7—C16—C15	1.3 (2)
O1—S1—C7—C16	62.39 (13)	S1—C7—C16—C15	−179.43 (14)
C16—C7—C8—C9	−0.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.93	2.51	3.424 (2)	169
C5—H5···*Cg*2^{ii}	0.93	2.96	3.486 (2)	117
C6—H6···*Cg*3^{ii}	0.93	2.94	3.535 (2)	123
C12—H12···*Cg*1^{iii}	0.93	2.94	3.788 (3)	152

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+3/2, −*y*+2, *z*+1/2; (iii) −*x*, *y*+5/2, −*z*+1/2.