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4-Aminophenyl naphthalene-1-sulfonate

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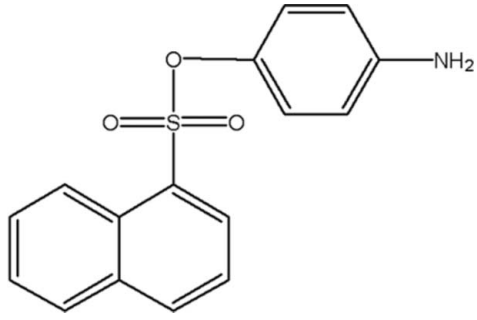
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.164; data-to-parameter ratio = 24.4.

In the title compound, $C_{16}H_{13}NO_3S$, the plane of the aminobenzene ring makes a dihedral angle of 61.04 (6)° with the naphthalene ring system. Both ring systems form weak intramolecular C—H···O hydrogen bonds with the sulfonate group. In the crystal structure, weak intermolecular N—H···O hydrogen bonds and a C—H···π interaction are observed.

Related literature

For biological activity, see: Yachi *et al.* (1989). For the structures of closely related compounds, see: Manivannan *et al.* (2005*a*,*b*).



Experimental

Crystal data

$C_{16}H_{13}NO_3S$
M_r = 299.33
Orthorhombic, $P2_12_12_1$
a = 7.0456 (3) Å
b = 12.4789 (6) Å
c = 15.8064 (8) Å
V = 1389.72 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
0.36 × 0.16 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.918, T_{max} = 0.962
19808 measured reflections
4629 independent reflections
3267 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.164
S = 1.03
4629 reflections
190 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Absolute structure: Flack (1983), 1972 Friedel pairs
Flack parameter: −0.01 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3	0.93	2.52	3.038 (3)	116
C8—H8···O3	0.93	2.38	2.804 (4)	108
C15—H15···O2	0.93	2.44	3.071 (4)	125
N1—H1B···O1^{i}	0.86	2.05	2.909 (3)	173
N1—H1A···O3^{ii}	0.86	1.94	2.773 (3)	162
C6—H6···Cg^{iii}	0.93	2.84	3.380 (3)	107

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$. *Cg* is the centroid of the C11–C16 ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2293).

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Yachi, K., Sugiyama, Y., Sawada, Y., Iga, T., Ikeda, Y., Toda, G. & Hananon, M. (1989). *Biochim. Biophys. Acta*, **978**, 1–7.

supporting information

Acta Cryst. (2008). E**64**, o1124 [doi:10.1107/S1600536808014438]

4-Aminophenyl naphthalene-1-sulfonate

Jasmine P. Vennila, R. Thilagavathi, R. Kavipriya, Helen P. Kavitha and V. Manivannan

S1. Comment

Several compounds containing *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).

We report the crystal structure of the title compound, (I). The geometric parameters of the molecule of (I) (Fig. 1) agree well with the reported structures (Manivannan *et al.* 2005*a*,*b*). The plane of the aminobenzene ring forms a dihedral angle of 61.04 (6)° with the naphthalene ring.

The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular N—H···O interactions and a C—H···π interaction (Table 1), involving the ring C11—C16 (centroid *Cg*).

S2. Experimental

1-Napthalene sulfonyl chloride (5 mmol) dissolved in acetone (4 ml) was added dropwise to *p*-amino phenol (5 mmol) in aqueous NaOH (4 ml, 5%) with constant shaking. The precipitated compound (3.5 mmol, yield 70%) was recrystlized from ethanol.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93 and N—H = 0.86 Å) and refined using riding model, with U_{iso}(H) = 1.2U_{eq}(C, N). The anisotropic displacement parameters of O1, S1 and C1 atoms were refined with a rigid bond restraint (DELU) in the final cycles of refinement.

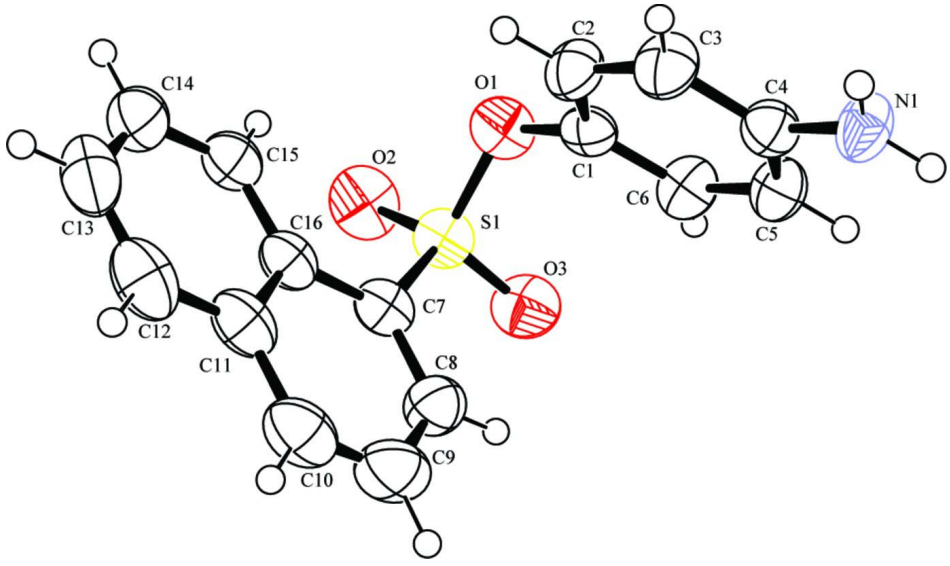

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Intramolecular H-bonds are shown as dotted lines.

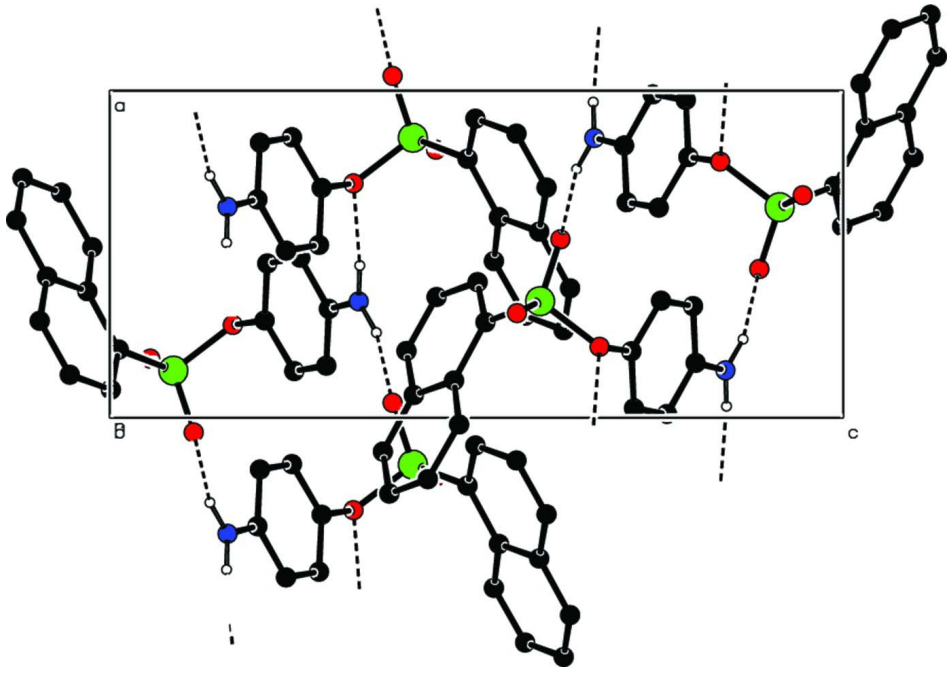

Figure 2

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.

4-Aminophenyl naphthalene-1-sulfonate

Crystal data

$C_{16}H_{13}NO_3S$
$M_r = 299.33$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.0456$ (3) Å
$b = 12.4789$ (6) Å
$c = 15.8064$ (8) Å
$V = 1389.72$ (11) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4586 reflections
$\theta = 2.8$–$25.7°$
$\mu = 0.24$ mm^{-1}
$T = 295$ K
Block, brown
0.36 × 0.16 × 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)
$T_{min} = 0.918$, $T_{max} = 0.962$
19808 measured reflections
4629 independent reflections
3267 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 31.9°$, $\theta_{min} = 2.1°$
$h = -10 \rightarrow 10$
$k = -18 \rightarrow 18$
$l = -23 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.164$
$S = 1.03$
4629 reflections
190 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2 + 0.1498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Absolute structure: Flack (1983), 1972 Friedel pairs
Absolute structure parameter: −0.01 (10)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2028 (3)	−0.04132 (18)	0.71108 (14)	0.0415 (4)
C2	0.0284 (3)	−0.0930 (2)	0.71475 (17)	0.0508 (6)
H2	−0.0763	−0.0641	0.6871	0.061*
C3	0.0110 (3)	−0.1874 (2)	0.7597 (2)	0.0545 (6)
H3	−0.1064	−0.2211	0.7637	0.065*
C4	0.1674 (3)	−0.23186 (18)	0.79873 (15)	0.0443 (5)
C5	0.3412 (3)	−0.18155 (19)	0.79520 (16)	0.0488 (5)
H5	0.4463	−0.2117	0.8217	0.059*
C6	0.3577 (3)	−0.08513 (19)	0.75158 (17)	0.0503 (5)
H6	0.4740	−0.0500	0.7497	0.060*
C7	0.2918 (4)	−0.0253 (2)	0.51224 (15)	0.0462 (5)
C8	0.4146 (4)	−0.1082 (2)	0.5015 (2)	0.0569 (6)

H8	0.5286	−0.1097	0.5311	0.068*
C9	0.3689 (6)	−0.1918 (2)	0.4455 (2)	0.0699 (8)
H9	0.4551	−0.2472	0.4370	0.084*
C10	0.2039 (6)	−0.1927 (2)	0.40449 (19)	0.0634 (7)
H10	0.1759	−0.2496	0.3685	0.076*
C11	0.0689 (4)	−0.1083 (2)	0.41450 (18)	0.0539 (6)
C12	−0.1042 (5)	−0.1111 (3)	0.3724 (2)	0.0664 (8)
H12	−0.1329	−0.1691	0.3377	0.080*
C13	−0.2326 (5)	−0.0302 (3)	0.38116 (19)	0.0685 (8)
H13	−0.3481	−0.0328	0.3527	0.082*
C14	−0.1884 (4)	0.0572 (3)	0.43368 (18)	0.0621 (7)
H14	−0.2748	0.1131	0.4393	0.074*
C15	−0.0212 (4)	0.0612 (2)	0.47630 (17)	0.0515 (6)
H15	0.0046	0.1198	0.5108	0.062*
C16	0.1133 (3)	−0.02101 (18)	0.46937 (15)	0.0451 (5)
N1	0.1446 (3)	−0.32773 (15)	0.83938 (13)	0.0487 (5)
H1A	0.2400	−0.3580	0.8635	0.058*
H1B	0.0348	−0.3578	0.8408	0.058*
O1	0.2166 (3)	0.05975 (15)	0.66776 (12)	0.0592 (5)
O2	0.3197 (4)	0.17748 (15)	0.55522 (14)	0.0706 (6)
O3	0.5453 (3)	0.04850 (19)	0.61441 (14)	0.0659 (6)
S1	0.35628 (9)	0.07323 (5)	0.58673 (4)	0.04995 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0433 (10)	0.0422 (9)	0.0391 (11)	−0.0016 (8)	−0.0002 (9)	−0.0121 (8)
C2	0.0377 (10)	0.0564 (14)	0.0584 (15)	−0.0005 (9)	−0.0021 (10)	0.0099 (12)
C3	0.0381 (10)	0.0611 (15)	0.0644 (16)	−0.0067 (10)	−0.0023 (10)	0.0090 (14)
C4	0.0447 (11)	0.0441 (11)	0.0440 (12)	−0.0009 (9)	0.0012 (9)	0.0003 (9)
C5	0.0444 (11)	0.0485 (12)	0.0535 (14)	−0.0027 (10)	−0.0119 (10)	−0.0009 (11)
C6	0.0442 (10)	0.0461 (12)	0.0607 (15)	−0.0082 (10)	−0.0094 (11)	−0.0036 (11)
C7	0.0534 (12)	0.0399 (11)	0.0452 (12)	−0.0093 (9)	0.0063 (10)	−0.0008 (10)
C8	0.0586 (14)	0.0531 (14)	0.0591 (17)	0.0050 (11)	0.0030 (13)	0.0016 (12)
C9	0.093 (2)	0.0475 (14)	0.0694 (19)	0.0115 (15)	0.0126 (18)	−0.0080 (14)
C10	0.088 (2)	0.0484 (14)	0.0536 (15)	−0.0082 (13)	0.0071 (15)	−0.0097 (13)
C11	0.0719 (15)	0.0475 (13)	0.0423 (13)	−0.0153 (11)	0.0063 (12)	−0.0005 (11)
C12	0.083 (2)	0.0687 (18)	0.0474 (15)	−0.0234 (16)	−0.0050 (14)	−0.0016 (14)
C13	0.0637 (17)	0.092 (2)	0.0500 (15)	−0.0171 (16)	−0.0091 (13)	0.0141 (17)
C14	0.0585 (14)	0.0730 (19)	0.0547 (15)	0.0032 (13)	0.0028 (12)	0.0103 (14)
C15	0.0569 (13)	0.0520 (14)	0.0456 (13)	−0.0040 (10)	0.0064 (10)	0.0026 (11)
C16	0.0550 (12)	0.0409 (11)	0.0395 (11)	−0.0095 (9)	0.0054 (10)	0.0018 (9)
N1	0.0379 (8)	0.0452 (10)	0.0631 (13)	−0.0036 (8)	−0.0047 (9)	0.0182 (9)
O1	0.0663 (10)	0.0520 (9)	0.0594 (10)	−0.0055 (8)	0.0036 (8)	−0.0032 (8)
O2	0.0897 (16)	0.0419 (10)	0.0803 (14)	−0.0233 (10)	0.0025 (12)	0.0052 (10)
O3	0.0465 (9)	0.0750 (14)	0.0763 (13)	−0.0157 (9)	0.0011 (9)	−0.0054 (11)
S1	0.0510 (3)	0.0416 (3)	0.0573 (4)	−0.0135 (2)	0.0011 (3)	−0.0021 (3)

Geometric parameters (Å, º)

C1—C6	1.378 (3)	C9—H9	0.9300
C1—C2	1.389 (3)	C10—C11	1.428 (5)
C1—O1	1.438 (3)	C10—H10	0.9300
C2—C3	1.381 (4)	C11—C12	1.390 (4)
C2—H2	0.9300	C11—C16	1.427 (3)
C3—C4	1.380 (3)	C12—C13	1.362 (5)
C3—H3	0.9300	C12—H12	0.9300
C4—N1	1.368 (3)	C13—C14	1.406 (5)
C4—C5	1.377 (3)	C13—H13	0.9300
C5—C6	1.392 (3)	C14—C15	1.358 (4)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.401 (4)
C7—C8	1.360 (4)	C15—H15	0.9300
C7—C16	1.430 (3)	N1—H1A	0.8600
C7—S1	1.762 (3)	N1—H1B	0.8600
C8—C9	1.404 (4)	O2—S1	1.417 (2)
C8—H8	0.9300	O3—S1	1.436 (2)
C9—C10	1.332 (5)	O1—S1	1.624 (2)
C6—C1—C2	119.8 (2)	C11—C10—H10	119.3
C6—C1—O1	121.0 (2)	C12—C11—C16	120.2 (3)
C2—C1—O1	119.1 (2)	C12—C11—C10	120.8 (3)
C3—C2—C1	119.7 (2)	C16—C11—C10	119.0 (3)
C3—C2—H2	120.1	C13—C12—C11	121.0 (3)
C1—C2—H2	120.1	C13—C12—H12	119.5
C4—C3—C2	120.1 (2)	C11—C12—H12	119.5
C4—C3—H3	119.9	C12—C13—C14	119.2 (3)
C2—C3—H3	119.9	C12—C13—H13	120.4
N1—C4—C5	121.5 (2)	C14—C13—H13	120.4
N1—C4—C3	117.9 (2)	C15—C14—C13	120.9 (3)
C5—C4—C3	120.6 (2)	C15—C14—H14	119.5
C4—C5—C6	119.2 (2)	C13—C14—H14	119.5
C4—C5—H5	120.4	C14—C15—C16	121.4 (3)
C6—C5—H5	120.4	C14—C15—H15	119.3
C1—C6—C5	120.5 (2)	C16—C15—H15	119.3
C1—C6—H6	119.8	C15—C16—C11	117.3 (2)
C5—C6—H6	119.8	C15—C16—C7	125.8 (2)
C8—C7—C16	121.9 (2)	C11—C16—C7	116.9 (2)
C8—C7—S1	116.8 (2)	C4—N1—H1A	120.0
C16—C7—S1	121.19 (19)	C4—N1—H1B	120.0
C7—C8—C9	119.9 (3)	H1A—N1—H1B	120.0
C7—C8—H8	120.1	C1—O1—S1	120.50 (15)
C9—C8—H8	120.1	O2—S1—O3	118.25 (13)
C10—C9—C8	120.9 (3)	O2—S1—O1	105.20 (13)
C10—C9—H9	119.6	O3—S1—O1	107.43 (12)
C8—C9—H9	119.6	O2—S1—C7	111.02 (13)

C9—C10—C11	121.4 (3)	O3—S1—C7	107.04 (13)
C9—C10—H10	119.3	O1—S1—C7	107.38 (11)
C6—C1—C2—C3	0.7 (4)	C14—C15—C16—C11	1.1 (4)
O1—C1—C2—C3	−176.8 (2)	C14—C15—C16—C7	−179.1 (2)
C1—C2—C3—C4	−1.9 (4)	C12—C11—C16—C15	−1.9 (4)
C2—C3—C4—N1	−177.2 (2)	C10—C11—C16—C15	178.9 (2)
C2—C3—C4—C5	1.6 (4)	C12—C11—C16—C7	178.3 (2)
N1—C4—C5—C6	178.7 (2)	C10—C11—C16—C7	−1.0 (3)
C3—C4—C5—C6	−0.1 (4)	C8—C7—C16—C15	−179.7 (3)
C2—C1—C6—C5	0.9 (4)	S1—C7—C16—C15	4.3 (3)
O1—C1—C6—C5	178.3 (2)	C8—C7—C16—C11	0.1 (3)
C4—C5—C6—C1	−1.1 (4)	S1—C7—C16—C11	−175.90 (18)
C16—C7—C8—C9	1.4 (4)	C6—C1—O1—S1	63.1 (3)
S1—C7—C8—C9	177.6 (2)	C2—C1—O1—S1	−119.4 (2)
C7—C8—C9—C10	−2.0 (5)	C1—O1—S1—O2	174.10 (17)
C8—C9—C10—C11	1.2 (5)	C1—O1—S1—O3	−59.1 (2)
C9—C10—C11—C12	−178.9 (3)	C1—O1—S1—C7	55.8 (2)
C9—C10—C11—C16	0.4 (4)	C8—C7—S1—O2	137.0 (2)
C16—C11—C12—C13	1.4 (4)	C16—C7—S1—O2	−46.8 (2)
C10—C11—C12—C13	−179.4 (3)	C8—C7—S1—O3	6.6 (2)
C11—C12—C13—C14	0.0 (4)	C16—C7—S1—O3	−177.21 (18)
C12—C13—C14—C15	−0.8 (4)	C8—C7—S1—O1	−108.5 (2)
C13—C14—C15—C16	0.3 (4)	C16—C7—S1—O1	67.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3	0.93	2.52	3.038 (3)	116
C8—H8···O3	0.93	2.38	2.804 (4)	108
C15—H15···O2	0.93	2.44	3.071 (4)	125
N1—H1*B*···O1^{i}	0.86	2.05	2.909 (3)	173
N1—H1*A*···O3^{ii}	0.86	1.94	2.773 (3)	162
C6—H6···*Cg*^{iii}	0.93	2.84	3.380 (3)	107

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