max. residual density 0·19, min. −0·14 e Å^{-3}, extinction coefficient (Larson, 1969) $g = 5{\cdot}0\,(4) \times 10^{-6}$ where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c, maximum correction 16·5% for the $30\bar{2}$ reflection. Table 1 presents the final coordinates* and equivalent isotropic thermal parameters, and Table 2 presents bond distances and angles. Fig. 1 illustrates the molecule and the numbering scheme; and Fig. 2 shows the unit cell.

Related literature. The space group of naphthalene-2,7-diol is discussed in Ahmed (1978). For macrocycles containing the 2,7-dioxynaphthyl group see Hamilton & Van Engen (1987) and Muehldorf, Van Engen, Warner & Hamilton (1988). For the crystal structure of 2,7-dimethoxynaphthalene see Prince, Fronczek & Gandour (1989*a*), for 1-acetyl-2,7-dimethoxynaphthalene see Prince, Fronczek & Gandour (1989*b*), for 1-(1-chlorovinyl)-2,7-dimethoxynaphthalene see Prince, Evans, Boss, Fronczek & Gandour (1990), and for 1-ethynyl-2,7-dimethoxynaphthalene see Prince, Fronczek & Gandour (1990).

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* Tables of H-atom coordinates, bond distances and angles involving H atoms, anisotropic thermal parameters, a table of least-squares planes, and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54124 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,7-Naphthalenediyl Bis(*p*-toluenesulfonate)

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Abstract. $C_{24}H_{20}O_6S_2$, $M_r = 468{\cdot}6$, triclinic, $P\bar{1}$, $a = 8{\cdot}4835\,(7)$, $b = 11{\cdot}801\,(2)$, $c = 12{\cdot}036\,(2)$ Å, $\alpha = 82{\cdot}321\,(10)$, $\beta = 76{\cdot}560\,(8)$, $\gamma = 73{\cdot}261\,(8)°$, $V = 1119{\cdot}4\,(3)$ Å^3, $Z = 2$, $D_x = 1{\cdot}390$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 24{\cdot}38$ cm^{-1}, $F(000) = 488$, $T = 296$ K, $R = 0{\cdot}037$ for 4025 observations having $I > 3\sigma(I)$ (of 4620 unique data). The average deviation from planarity is 0·018 (2) Å with a maximum of 0·034 (1) Å for the fused rings. One of the toluenesulfonate groups points towards the neighboring α-carbon of the ring, whereas the second one points in the opposite direction forming C—O—S—C torsion angles −79·96 (12) and +81·10 (11)°. The dihedral angles between the naphthalene system and the toluenesulfonyl rings are 74·20 (5) and 134·40 (4)° respectively. The S—C distances are 1·743 (2) and 1·753 (1) Å, the S—O distances are identical with length 1·601 (1) Å, and the S=O distances range 1·415 (1)–1·424 (1) Å.

Experimental. Colorless crystals of (1), m.p. 425–426 K, were isolated by recrystallization from THF/hexane of the crude reaction product of 2,7-dihydroxynaphthalene and toluene-4-sulfonyl chloride in dichloromethane/pyridine at 278 K. Crystal size 0·10 × 0·32 × 0·48 mm, mounted on a glass fiber in random orientation on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator, Cu $K\alpha$ radiation. Cell dimensions from setting angles of 25 reflections having $25 < \theta <$

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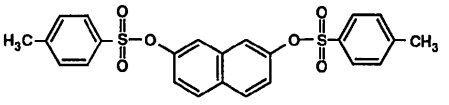
30°. Successful refinement of a centrosymmetric model determined the space group as $P\bar{1}$.



(1)

A full sphere of data having $2 < \theta < 75°$, $-10 \le h \le 10$, $-13 \le k \le 14$, $-14 \le l \le 14$ was measured using ω–2θ scans designed for $I = 50\sigma(I)$, subject to max. scan time = 120 s, scan rates varied 0·57–3·30° min^{-1}. Data corrected for background, Lorentz and polarization effects. Intensities of standard reflections (500, 030, 006) decreased 2·3%, and a linear decay correction was applied. Absorption corrections were based on ψ scans, and relative transmission coefficients ranged from 0·633 to 0·998 with an average value of 0·872. A total of 9032 data was measured. $R_{int} = 0{\cdot}016$ for averaging the two redundant hemispheres. Structure solved by direct methods, using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). The structure was refined by weighted full-matrix least squares; non-H atoms refined anisotropically; H atoms located by ΔF and refined isotropically.

The function minimized was $\sum w(|F_o| - |F_o|)^2$ and weights were assigned as $w = 4F_o^2\mathrm{Lp}[S^2(C + R^2B) + (0{\cdot}02F_o^2)^2]^{-1}$, where S = scan rate, C = total integrated peak count, R = scan time/background counting time, B = total background count, Lp = Lorentz–polarization factor, using Enraf–Nonius *SDP* (Frenz & Okaya, 1980), scattering factors of Cromer & Waber (1974), anomalous coefficients of Cromer (1974). Of 4620 unique data, 4025 reflections having $I > 3\sigma(I)$ were used in the refinement. Final $R = 0{\cdot}037$ (0·042 for all data), $wR = 0{\cdot}056$, $S = 2{\cdot}880$ for 370 variables. Max. shift $0{\cdot}30\sigma$ in the final cycle; $0{\cdot}01\sigma$ for a non-H atom, max. residual density 0·30, min. −0·33 e Å^{-3}. The extinction coefficient was refined in the least squares to $g = 3{\cdot}1\ (3) \times 10^{-6}$ where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c. The intensities of the strongest reflections ($02\bar{1}$ and 221) were affected by 20%. Table 1* presents the final coordinates and equivalent isotropic thermal parameters, Table 2 presents bond distances and angles. Fig. 1 illustrates the molecule and the numbering scheme, and Fig. 2 shows the unit cell.

* Lists of H-atom coordinates, bond distances and angles involving H atoms, torsion angles, anisotropic thermal parameters, least-squares planes and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54106 (30 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Coordinates and equivalent isotropic thermal parameters*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
S1	0·31557 (5)	0·40685 (3)	0·38225 (4)	5·132 (9)
S2	0·88225 (5)	0·99781 (3)	0·17912 (3)	4·465 (7)
O1	0·2735 (1)	0·54638 (9)	0·39484 (9)	4·74 (2)
O2	0·2621 (2)	0·3624 (1)	0·4957 (1)	7·56 (3)
O3	0·4855 (2)	0·3668 (1)	0·3237 (2)	7·24 (4)
O4	0·8986 (1)	0·86695 (9)	0·14730 (9)	4·29 (2)
O5	1·0494 (2)	1·0082 (1)	0·1416 (1)	6·33 (3)
O6	0·7480 (2)	1·0804 (1)	0·1352 (1)	5·62 (3)
C1	0·4853 (2)	0·6462 (1)	0·3118 (1)	3·96 (3)
C2	0·3447 (2)	0·6173 (1)	0·3037 (1)	3·89 (3)
C3	0·2605 (2)	0·6608 (1)	0·2131 (1)	4·33 (3)
C4	0·3253 (2)	0·7328 (1)	0·1273 (1)	4·29 (3)
C5	0·5387 (2)	0·8412 (1)	0·0430 (1)	4·24 (3)
C6	0·6770 (2)	0·8754 (1)	0·0489 (1)	4·25 (3)
C7	0·7514 (2)	0·8343 (1)	0·1449 (1)	3·70 (3)
C8	0·6952 (2)	0·7593 (1)	0·2304 (1)	3·78 (3)
C9	0·5527 (2)	0·7224 (1)	0·2249 (1)	3·52 (3)
C10	0·4721 (2)	0·7651 (1)	0·1302 (1)	3·70 (3)
C11	0·1810 (2)	0·3959 (1)	0·2970 (1)	4·37 (3)
C12	0·0138 (2)	0·4062 (2)	0·3460 (1)	5·21 (4)
C13	−0·0936 (2)	0·3972 (2)	0·2796 (2)	6·14 (4)
C14	−0·0374 (3)	0·3787 (2)	0·1649 (2)	6·09 (4)
C15	0·1296 (3)	0·3710 (2)	0·1165 (2)	6·57 (5)
C16	0·2416 (3)	0·3778 (2)	0·1818 (2)	5·60 (4)
C17	−0·1552 (3)	0·3671 (2)	0·0937 (2)	9·85 (6)
C18	0·8279 (2)	0·9885 (1)	0·3291 (1)	4·00 (3)
C19	0·6950 (2)	1·0733 (2)	0·3841 (2)	5·43 (4)
C20	0·6544 (3)	1·0658 (2)	0·5020 (2)	6·05 (5)
C21	0·7446 (2)	0·9748 (1)	0·5660 (1)	4·78 (3)
C22	0·8793 (2)	0·8935 (1)	0·5094 (1)	4·87 (4)
C23	0·9235 (2)	0·8984 (2)	0·3911 (1)	4·81 (4)
C24	0·6945 (3)	0·9641 (2)	0·6957 (2)	6·76 (5)

Table 2. *Bond distances* (Å) *and angles* (°)

S1	O1	1·601 (1)		C7	C8	1·356 (2)	
S1	O2	1·415 (1)		C8	C9	1·416 (2)	
S1	O3	1·422 (1)		C9	C10	1·425 (2)	
S1	C11	1·743 (2)		C11	C12	1·381 (2)	
S2	O4	1·600 (1)		C11	C16	1·385 (2)	
S2	O5	1·420 (1)		C12	C13	1·378 (3)	
S2	O6	1·424 (1)		C13	C14	1·376 (3)	
S2	C18	1·753 (1)		C14	C15	1·382 (3)	
O1	C2	1·416 (2)		C14	C17	1·503 (4)	
O4	C7	1·417 (2)		C15	C16	1·391 (4)	
C1	C2	1·358 (2)		C18	C19	1·375 (2)	
C1	C9	1·413 (2)		C18	C23	1·384 (2)	
C2	C3	1·402 (2)		C19	C20	1·378 (3)	
C3	C4	1·364 (2)		C20	C21	1·382 (2)	
C4	C10	1·412 (2)		C21	C22	1·368 (2)	
C5	C6	1·365 (3)		C21	C24	1·518 (2)	
C5	C10	1·411 (2)		C22	C23	1·383 (2)	
C6	C7	1·408 (2)					
O1	S1	O2	102·64 (7)	C7	C8	C9	118·9 (1)
O1	S1	O3	108·50 (8)	C1	C9	C8	122·0 (1)
O1	S1	C11	103·96 (7)	C1	C9	C10	118·7 (1)
O2	S1	O3	120·72 (9)	C8	C9	C10	119·3 (1)
O2	S1	C11	109·71 (9)	C4	C10	C5	121·6 (1)
O3	S1	C11	109·80 (9)	C4	C10	C9	119·3 (1)
O4	S2	O5	102·69 (7)	C5	C10	C9	119·1 (1)
O4	S2	O6	109·80 (7)	S1	C11	C12	119·0 (1)
O4	S2	C18	103·45 (6)	S1	C11	C16	120·2 (1)
O5	S2	O6	120·28 (8)	C12	C11	C16	120·8 (2)
O5	S2	C18	110·30 (8)	C11	C12	C13	119·5 (2)
O6	S2	C18	108·91 (6)	C12	C13	C14	121·1 (2)
S1	O1	C2	118·55 (8)	C13	C14	C15	118·7 (2)
S2	O4	C7	119·27 (8)	C13	C14	C17	120·6 (2)
C2	C1	C9	119·3 (1)	C15	C14	C17	120·7 (2)
O1	C2	C1	118·4 (1)	C14	C15	C16	121·5 (2)
O1	C2	C3	118·4 (1)	C11	C16	C15	118·3 (2)
C1	C2	C3	123·0 (1)	S2	C18	C19	119·7 (1)
C2	C3	C4	118·6 (2)	S2	C18	C23	119·6 (1)
C3	C4	C10	121·0 (1)	C19	C18	C23	120·7 (1)
C6	C5	C10	121·1 (1)	C18	C19	C20	119·2 (2)
C5	C6	C7	118·5 (1)	C19	C20	C21	121·3 (2)
O4	C7	C6	117·7 (1)	C20	C21	C22	118·3 (1)
O4	C7	C8	119·0 (1)	C20	C21	C24	121·0 (1)
C6	C7	C8	123·1 (2)	C22	C21	C24	120·7 (1)
C21	C22	C23	121·8 (1)	C18	C23	C22	118·6 (1)

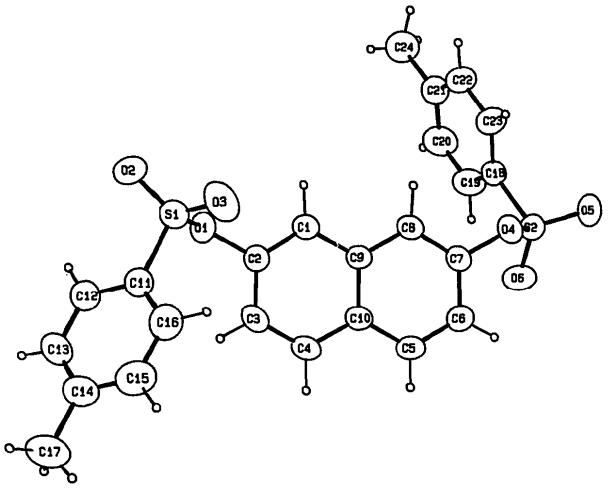


Fig. 1. Numbering scheme and thermal ellipsoids drawn at the 40% probability level. H atoms are drawn as circles of arbitrary radius.

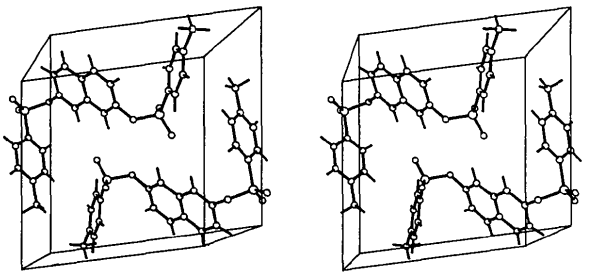


Fig. 2. Stereoview of the unit cell. **a** is into the plane of the paper, **b** is horizontal and **c** is vertical.

Related literature. Crystal structures of other aromatic toluenesulfonates: tetrachloro-*p*-phenylene bis(*p*-toluenesulfonate) (Wieczorek & Galdecki, 1978), tetramethyl-*p*-phenylene bis(*p*-toluenesulfonate (Wieczorek, Bokiy & Struchkov, 1975), 2-tosyloxy-5-methylisophthalaldehyde (Sarkar & Gupta, 1980) and tetrabromo-*p*-phenylene bis(*p*-toluenesulfonate) (Wieczorek, 1980).

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(Formyl-2 pyrrolyl-1)-2 Thiophenecarbonitrile-3

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Abstract. $C_{10}H_6N_2OS$, $M_r = 202{\cdot}22$, monoclinic, $P2/n$ (first setting), $a = 13{\cdot}039$ (4), $b = 7{\cdot}317$ (2), $c = 9{\cdot}995$ (4) Å, $\gamma = 104{\cdot}37$ (2)°, $V = 923{\cdot}7$ (1) Å^3, $Z = 4$, $D_m = 1{\cdot}46$, $D_x = 1{\cdot}45$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}31$ mm^{-1}, $F(000) = 416$, room temperature, $R = 0{\cdot}043$ for 770 independent reflections [$I > 3\sigma(I)$]. The title compound is built up of one pyrrole ring and one thiophene ring, the dihedral

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