Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Hydroxyphenylsulfonyl)phenol

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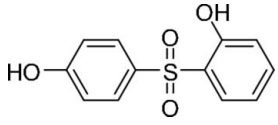
Received 30 December 2008; accepted 21 January 2009

Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.162; data-to-parameter ratio = 12.3.

The title compound, $C_{12}H_{10}O_4S$, is a phenolic color developer used for leuco colorants. The two benzene rings with substituent hydroxy groups are nearly perpendicular to each other [dihedral angle = 91.5 (1)°]. There are intermolecular O—H···O hydrogen bonds between an OH group of one molecule and a sulfonyl O atom of a neighboring molecule. One molecule is hydrogen bonded to four symmetry-related molecules, forming a two-dimensional hydrogen-bond network.

Related literature

For general background literature on leuco dyes, see: Muthyala (1997). For the structure of 4,4′-sulfonyldiphenol, see: Glidewell & Ferguson (1996); Davies *et al.* (1997).



Experimental

Crystal data

$C_{12}H_{10}O_4S$
M_r = 250.27
Monoclinic, $P2_1/c$
a = 10.9525 (2) Å
b = 14.4404 (3) Å
c = 7.0361 (1) Å
β = 93.8147 (10)°
V = 1110.35 (3) Å^3
Z = 4
Cu- $K\alpha$ radiation
μ = 2.62 mm^{-1}
T = 93.1 K
0.39 × 0.35 × 0.29 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.408, T_{max} = 0.468
9436 measured reflections
1998 independent reflections
1830 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.154

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.162
S = 1.10
1998 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O2^{i}	0.87 (3)	1.90 (3)	2.753 (2)	168 (3)
O4—H4O···O1^{ii}	0.88 (4)	1.85 (4)	2.733 (2)	173 (3)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2215).

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supporting information

Acta Cryst. (2009). E**65**, o391 [doi:10.1107/S160053680900258X]

2-(4-Hydroxyphenylsulfonyl)phenol

Kazuyuki Sato, Hideki Shima and Jin Mizuguchi

S1. Comment

The colorless leuco dye is known to exhibit a brilliant color when the lactone-ring is opened by the formation of intermolecular hydrogen bonds between dye and developer, and is used in practice in thermal or rewritable papers (Muthyala, 1997). The title compound has found use as a developer for fluoran leuco dyes which give a black color. Since the color is generated by a solid state reaction by heating a mixture of dye and developer particles, the mutual geometrical relation of dye and developer molecules plays an important role in color strength in the solid state. For this reason, structure analysis of 2-[4-hydroxyphenyl]sulfonyl]-phenol, (I), has been carried out in the present investigation.

Figure 1 shows the *ORTEPIII* plot (Burnett & Johnson, 1996) of (I). The two benzene rings with 2-hydroxy or 4-hydroxy group are nearly perpendicular to each other [dihedral angle: 91.5 (1)°]. Figure 2 is the projection of the crystal structure onto the (*b,c*) plane. There are O—H···O intermolecular hydrogen bonds between the OH of one molecule and the sulfonyl O atom of the neighboring one along the *b* and *c* axes. One molecule is hydrogen-bonded to four different molecules, forming a two-dimensional hydrogen-bond network. A similar two-dimensional network is found in 4,4′-sulfonyldiphenol (Glidewell & Ferguson, 1996; Davies *et al.*, 1997).

S2. Experimental

Compound (I) was obtained from Mitsubisihi Paper Mills., Ltd., and was recrystallized from an ethanol solution. After 48 h., a number of colorless crystals were obtained in the form of blocks.

S3. Refinement

The H atoms of the hydroxy groups (H3O and H4O) were found in density maps and refined isotropically. All other H atoms were positioned geometrically and included in the riding-model approximation, with C—H distances of 0.95 Å, and U_{iso}(H) = 1.2U_{eq}(C).

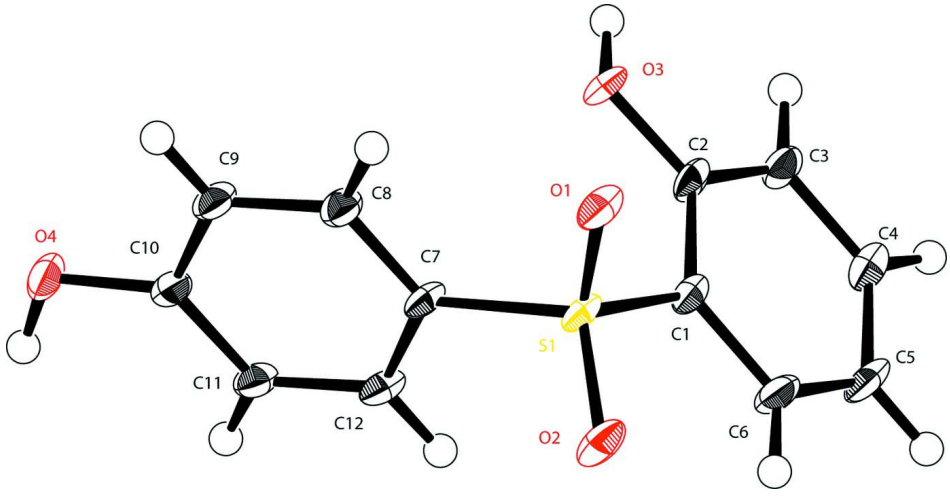

Figure 1

A view of the molecular structure of (I), showing 50% probability displacement ellipsoids for non-H atoms.

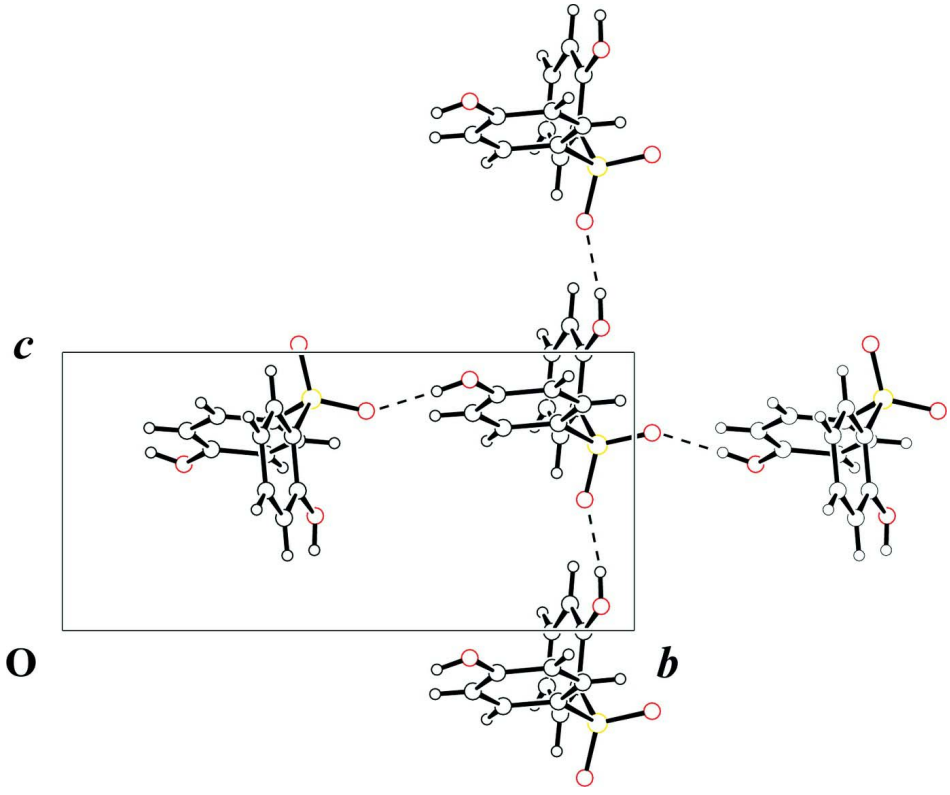

Figure 2

Projection of the structure of (I) onto the *b* and *c* plane, showing O—H···O intermolecular hydrogen bonds in dotted lines. One molecule is hydrogen-bonded to four different molecules along the *b* and *c* axes.

2-(4-Hydroxyphenylsulfonyl)phenol

Crystal data

$C_{12}H_{10}O_4S$
$M_r = 250.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.9525$ (2) Å
$b = 14.4404$ (3) Å
$c = 7.0361$ (1) Å
$\beta = 93.8147$ (10)°
$V = 1110.35$ (3) Å^3
$Z = 4$
$F(000) = 520.00$
$D_x = 1.497$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å
Cell parameters from 9882 reflections
$\theta = 3.1$–$68.2°$
$\mu = 2.62$ mm^{-1}
$T = 93$ K
Block, colorless
0.39 × 0.35 × 0.29 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.408$, $T_{max} = 0.468$
9436 measured reflections
1998 independent reflections
1830 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.154$
$\theta_{max} = 68.2°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.162$
$S = 1.10$
1998 reflections
163 parameters
0 restraints
0 constraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 1.2611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0.0078 (10)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.27104 (6)	0.93583 (5)	0.66743 (9)	0.0192 (2)
O1	0.30244 (18)	1.03113 (13)	0.7107 (3)	0.0240 (5)
O2	0.23614 (19)	0.91341 (15)	0.4710 (2)	0.0272 (5)
O3	0.25813 (18)	0.94202 (14)	1.0879 (2)	0.0217 (4)
O4	0.70235 (18)	0.71229 (14)	0.9019 (3)	0.0253 (5)
C1	0.1463 (2)	0.90270 (18)	0.7994 (3)	0.0184 (5)
C2	0.1531 (2)	0.91128 (18)	0.9972 (4)	0.0201 (6)
C3	0.0508 (2)	0.8876 (2)	1.0952 (4)	0.0222 (6)
C4	−0.0549 (2)	0.8560 (2)	0.9967 (4)	0.0243 (6)
C5	−0.0613 (2)	0.8473 (2)	0.7997 (4)	0.0265 (6)
C6	0.0399 (2)	0.8704 (2)	0.7008 (4)	0.0243 (6)
C7	0.3959 (2)	0.86727 (19)	0.7456 (3)	0.0192 (5)
C8	0.5037 (2)	0.90989 (19)	0.8143 (4)	0.0209 (6)
C9	0.6055 (2)	0.85644 (19)	0.8666 (4)	0.0218 (6)

C10	0.5990 (2)	0.76019 (19)	0.8485 (3)	0.0199 (6)
C11	0.4904 (2)	0.71764 (18)	0.7819 (3)	0.0204 (6)
C12	0.3887 (2)	0.77072 (19)	0.7286 (3)	0.0213 (6)
H3O	0.257 (3)	0.940 (2)	1.212 (5)	0.023 (8)*
H4O	0.695 (4)	0.653 (3)	0.862 (6)	0.058 (12)*
H3	0.0535	0.8933	1.2300	0.025*
H4	−0.1237	0.8395	1.0653	0.027*
H5	−0.1341	0.8255	0.7318	0.028*
H6	0.0369	0.8644	0.5664	0.027*
H8	0.5071	0.9755	0.8264	0.022*
H9	0.6792	0.8851	0.9143	0.025*
H11	0.4865	0.6518	0.7720	0.023*
H12	0.3143	0.7422	0.6813	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0162 (4)	0.0227 (4)	0.0174 (4)	−0.0020 (2)	−0.0079 (2)	0.0010 (2)
O1	0.0209 (10)	0.0219 (10)	0.0280 (10)	−0.0042 (7)	−0.0088 (8)	0.0019 (8)
O2	0.0222 (11)	0.0383 (11)	0.0199 (10)	−0.0033 (8)	−0.0087 (8)	0.0052 (9)
O3	0.0172 (10)	0.0281 (10)	0.0185 (10)	−0.0040 (7)	−0.0089 (8)	−0.0000 (8)
O4	0.0167 (10)	0.0220 (10)	0.0359 (11)	0.0023 (7)	−0.0089 (8)	−0.0010 (9)
C1	0.0140 (12)	0.0198 (12)	0.0206 (13)	−0.0011 (9)	−0.0050 (10)	0.0013 (11)
C2	0.0167 (13)	0.0180 (12)	0.0240 (14)	0.0030 (10)	−0.0100 (10)	0.0040 (11)
C3	0.0193 (13)	0.0265 (13)	0.0197 (13)	0.0024 (10)	−0.0071 (10)	0.0018 (11)
C4	0.0169 (13)	0.0278 (14)	0.0273 (15)	−0.0001 (10)	−0.0056 (10)	0.0028 (12)
C5	0.0186 (14)	0.0295 (15)	0.0295 (15)	−0.0054 (11)	−0.0123 (11)	−0.0008 (12)
C6	0.0211 (14)	0.0299 (14)	0.0204 (13)	−0.0023 (11)	−0.0091 (10)	−0.0026 (12)
C7	0.0172 (13)	0.0230 (13)	0.0160 (12)	−0.0017 (10)	−0.0081 (10)	0.0002 (11)
C8	0.0190 (14)	0.0189 (12)	0.0240 (14)	−0.0028 (10)	−0.0039 (10)	−0.0024 (11)
C9	0.0188 (14)	0.0204 (13)	0.0251 (14)	−0.0042 (10)	−0.0064 (10)	−0.0032 (11)
C10	0.0191 (13)	0.0213 (13)	0.0186 (12)	−0.0001 (10)	−0.0049 (10)	−0.0026 (11)
C11	0.0216 (14)	0.0181 (12)	0.0206 (13)	−0.0031 (10)	−0.0050 (10)	−0.0032 (10)
C12	0.0206 (13)	0.0222 (13)	0.0201 (13)	−0.0057 (10)	−0.0063 (10)	−0.0024 (11)

Geometric parameters (Å, º)

S1—O1	1.446 (2)	C4—H4	0.952
S1—O2	1.446 (2)	C5—C6	1.388 (4)
S1—C1	1.768 (2)	C5—H5	0.955
S1—C7	1.747 (2)	C6—H6	0.948
O3—C2	1.353 (3)	C7—C8	1.389 (3)
O3—H3O	0.87 (3)	C7—C12	1.401 (3)
O4—C10	1.358 (3)	C8—C9	1.386 (3)
O4—H4O	0.90 (4)	C8—H8	0.951
C1—C2	1.395 (3)	C9—C10	1.397 (3)
C1—C6	1.396 (3)	C9—H9	0.948
C2—C3	1.397 (4)	C10—C11	1.392 (3)

C3—C4	1.386 (3)	C11—C12	1.383 (3)
C3—H3	0.950	C11—H11	0.953
C4—C5	1.389 (4)	C12—H12	0.953
O1···O4^{i}	2.733 (2)	O3···H8^{ii}	2.862
O1···H4O^{i}	1.84 (4)	O3···H9^{ii}	2.590
O1···H9^{ii}	2.898	O3···H12^{v}	2.799
O1···H11^{i}	2.891	O4···O1^{vi}	2.733 (2)
O2···O3^{iii}	2.753 (2)	O4···H4^{vii}	2.835
O2···H3O^{iii}	1.89 (3)	O4···H5^{vii}	2.757
O2···H3^{iii}	2.552	O4···H5^{viii}	2.888
O3···O2^{iv}	2.753 (2)	C4···H9^{ix}	2.962
O1—S1—O2	117.29 (12)	C6—C5—H5	119.7
O1—S1—C1	109.16 (12)	C1—C6—C5	119.9 (2)
O1—S1—C7	107.63 (12)	C1—C6—H6	119.9
O2—S1—C1	106.08 (12)	C5—C6—H6	120.2
O2—S1—C7	108.99 (12)	S1—C7—C8	119.2 (2)
C1—S1—C7	107.30 (12)	S1—C7—C12	119.9 (2)
C2—O3—H3O	113 (2)	C8—C7—C12	120.8 (2)
C10—O4—H4O	110 (2)	C7—C8—C9	119.7 (2)
S1—C1—C2	120.6 (2)	C7—C8—H8	120.0
S1—C1—C6	118.6 (2)	C9—C8—H8	120.3
C2—C1—C6	120.9 (2)	C8—C9—C10	119.6 (2)
O3—C2—C1	119.1 (2)	C8—C9—H9	120.1
O3—C2—C3	122.2 (2)	C10—C9—H9	120.2
C1—C2—C3	118.7 (2)	O4—C10—C9	116.4 (2)
C2—C3—C4	120.3 (2)	O4—C10—C11	123.1 (2)
C2—C3—H3	119.9	C9—C10—C11	120.5 (2)
C4—C3—H3	119.8	C10—C11—C12	120.1 (2)
C3—C4—C5	120.9 (2)	C10—C11—H11	119.8
C3—C4—H4	119.4	C12—C11—H11	120.1
C5—C4—H4	119.6	C7—C12—C11	119.3 (2)
C4—C5—C6	119.3 (2)	C7—C12—H12	120.1
C4—C5—H5	120.9	C11—C12—H12	120.6
O1—S1—C1—C2	−55.8 (2)	C6—C1—C2—C3	−0.5 (3)
O1—S1—C1—C6	122.4 (2)	O3—C2—C3—C4	−179.7 (2)
O1—S1—C7—C8	−6.2 (2)	C1—C2—C3—C4	0.1 (3)
O1—S1—C7—C12	177.4 (2)	C2—C3—C4—C5	0.0 (3)
O2—S1—C1—C2	177.0 (2)	C3—C4—C5—C6	0.1 (3)
O2—S1—C1—C6	−4.9 (2)	C4—C5—C6—C1	−0.4 (4)
O2—S1—C7—C8	122.0 (2)	S1—C7—C8—C9	−176.4 (2)
O2—S1—C7—C12	−54.5 (2)	S1—C7—C12—C11	176.7 (2)
C1—S1—C7—C8	−123.5 (2)	C8—C7—C12—C11	0.3 (4)
C1—S1—C7—C12	60.0 (2)	C12—C7—C8—C9	0.1 (3)
C7—S1—C1—C2	60.6 (2)	C7—C8—C9—C10	0.4 (4)
C7—S1—C1—C6	−121.3 (2)	C8—C9—C10—O4	179.8 (2)

S1—C1—C2—O3	−2.5 (3)	C8—C9—C10—C11	−1.3 (4)
S1—C1—C2—C3	177.6 (2)	O4—C10—C11—C12	−179.6 (2)
S1—C1—C6—C5	−177.5 (2)	C9—C10—C11—C12	1.6 (4)
C2—C1—C6—C5	0.6 (4)	C10—C11—C12—C7	−1.1 (4)
C6—C1—C2—O3	179.4 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···O2^{iv}	0.87 (3)	1.90 (3)	2.753 (2)	168 (3)
O4—H4*O*···O1^{vi}	0.88 (4)	1.85 (4)	2.733 (2)	173 (3)

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