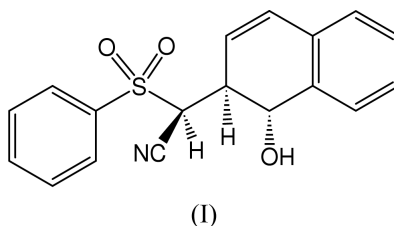


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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.048
 wR factor = 0.129
Data-to-parameter ratio = 12.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Benzenesulfonyl(1-hydroxy-1,2-dihydro-
naphthalen-2-yl)acetonitrileThe regiochemistry and relative stereochemistry of the title
compound, $\text{C}_{18}\text{H}_{15}\text{NO}_3\text{S}$, have been established. Molecules
form centrosymmetric hydrogen-bonded pairs *via* intermolecu-
lar $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds [$\text{H}\cdots\text{O}$ 2.01 (3) Å and $\text{O}-$
 $\text{H}\cdots\text{O}$ 168 (3) $^\circ$].Received 19 April 2002
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Comment

Recently, we reported a new rhodium-catalysed ring-opening
reaction of 1,4-dihydro-1,4-epoxynaphthalene with a wide
range of nucleophiles (Lautens & Fagnou, 2001). The 1,2-
regiochemistry and the *trans* relative stereochemistry were
established by the X-ray diffraction analysis when benzenesulfonylacetonitrile is used as the nucleophile.Molecules of the title compound, (I), form centrosymmetric
hydrogen-bonded pairs *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$
hydrogen bonds (see Fig. 1 and Table 2). In the dihydro-
naphthalene group, an analysis (Cremer & Pople, 1975) of the
puckering in the six-membered ring (C1–C5/C10) gives $Q_T =$
0.430 (2) Å. The conformational analysis of that ring (Duax *et*
al., 1976) shows that the conformation is half-chair, with a
local pseudo-twofold axis running through the midpoints of
the C1–C2 and C4–C5 bonds.

Experimental

The title compound was obtained as a mixture of the two
diastereomers as a colourless oil in 95% yield by treatment of 1,4-
dihydro-1,4-epoxynaphthalene with benzenesulfonylacetonitrile and
a catalyst prepared *in situ* from $[\text{Rh}(\text{cyclooctadiene})\text{Cl}]_2$ and bis-
(diphenylphosphino)ferrocene in refluxing tetrahydrofuran. The oil
was allowed to stand at room temperature for several weeks, during
which time the title compound gradually formed suitable crystals.

Crystal data

 $\text{C}_{18}\text{H}_{15}\text{NO}_3\text{S}$
 $M_r = 325.37$
Orthorhombic, *Pbcn*
 $a = 10.6135$ (6) Å
 $b = 12.6606$ (8) Å
 $c = 23.3280$ (16) Å
 $V = 3134.7$ (3) Å 3
 $Z = 8$
 $D_x = 1.379$ Mg m $^{-3}$ Mo $K\alpha$ radiation
Cell parameters from 2933
reflections
 $\theta = 2.6$ – 25.0°
 $\mu = 0.22$ mm $^{-1}$
 $T = 150$ (1) K
Block, colourless
 $0.20 \times 0.20 \times 0.18$ mm

Data collection

Nonius Kappa-CCD diffractometer
 φ scans, and ω scans with κ offsets
 Absorption correction: none
 10898 measured reflections
 2753 independent reflections
 2278 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -12 \rightarrow 12$
 $k = -15 \rightarrow 15$
 $l = -27 \rightarrow 27$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.129$
 $S = 1.10$
 2753 reflections
 213 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 2.8166P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.55 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXTL*
 Extinction coefficient: 0.0112 (17)

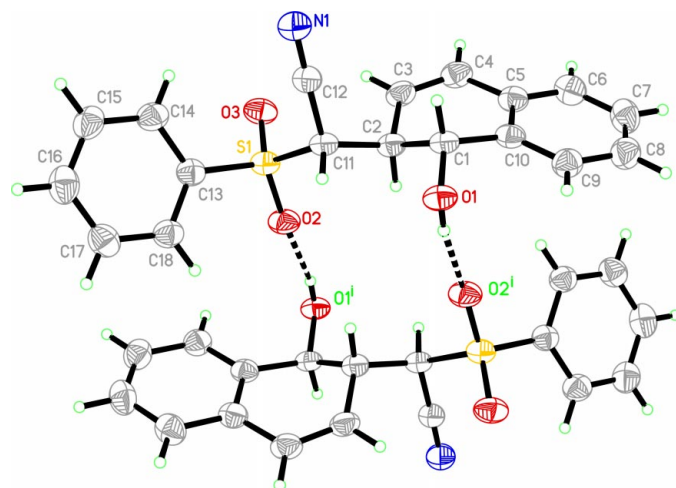


Figure 1

View of a hydrogen-bonded pair of the title molecule. Ellipsoids are shown at the 30% probability level. [Symmetry code: (i) $-x, 1-y, 1-z$.]

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1—C13	1.755 (3)	N1—C12	1.146 (3)
S1—C11	1.816 (3)	C3—C4	1.327 (4)
O1—C1	1.425 (3)	C11—C12	1.476 (3)
C13—S1—C11	106.61 (12)	N1—C12—C11	177.9 (3)
C2—C11—S1	111.73 (17)	C11—S1—C13—C18	−96.6 (2)
C13—S1—C11—C12	−64.16 (19)	C11—S1—C13—C14	86.8 (2)
C13—S1—C11—C2	171.59 (16)		

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1O \cdots O2 ⁱ	0.82 (3)	2.01 (3)	2.816 (3)	168 (3)

Symmetry code: (i) $-x, 1-y, 1-z$.

H atoms attached to C atoms were placed in calculated positions, with C—H distances ranging from 0.95 to 1.00 \AA , and were included in the refinement in riding-motion approximation, with $U_{\text{iso}} = 1.2U_{\text{eq}}$ of the carrier atom. The hydroxyl H atom was refined independently with an isotropic displacement parameter.

Data collection: *COLLECT* (Nonius, 1997–2001); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction:

DENZO-SMN; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

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