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## Structure Reports

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## *N'*-[1-(2-Hydroxyphenyl)ethylidene]-benzenesulfonohydrazide

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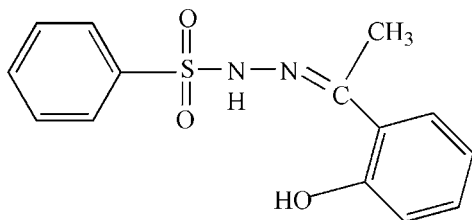
Received 19 April 2008; accepted 19 April 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.132; data-to-parameter ratio = 13.6.

In the title compound,  $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3\text{S}$ , the conformation is stabilized by an intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond and the dihedral angle between the aromatic ring planes is  $79.55(18)^\circ$ . In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds lead to [100] chains of molecules.

### Related literature

For related literature, see: Tai *et al.* (2003).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3\text{S}$   
 $M_r = 290.33$

Monoclinic,  $P2_1/n$   
 $a = 5.2435(9)$  Å

$b = 13.2515(18)$  Å  
 $c = 20.375(2)$  Å  
 $\beta = 90.531(2)^\circ$   
 $V = 1415.7(3)$  Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.24$  mm<sup>-1</sup>  
 $T = 298(2)$  K  
 $0.50 \times 0.40 \times 0.37$  mm

#### Data collection

Bruker SMART CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.891$ ,  $T_{\max} = 0.918$

7165 measured reflections  
2484 independent reflections  
1755 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.131$   
 $S = 1.04$   
2484 reflections

182 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.26$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3}\cdots\text{N2}$	0.82	1.85	2.561(3)	145
$\text{N1}-\text{H1}\cdots\text{O2}^{\dagger}$	0.90	2.20	3.093(3)	174

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors thank the National Natural Science Foundation of China (20671073), the Natural Science Foundation of Shandong (Y2007B60), and the Science and Technology Foundation of Weifang University for research grants.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2723).

### References

- Bruker (2000). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Tai, X. S., Yin, X. H., Tan, M. Y. & Li, Y. Z. (2003). *Acta Cryst.* **E59**, o681–o682.

**supplementary materials**

*Acta Cryst.* (2008). E64, o904 [ doi:10.1107/S1600536808010970 ]

## *N'*-[1-(2-Hydroxyphenyl)ethylidene]benzenesulfonohydrazide

X.-S. Tai, J. Xu, Y.-M. Feng and Z.-P. Liang

### Comment

As part of our ongoing studies of the coordination chemistry of aroylhydrazones as potential ligands (Tai *et al.*, 2003), we now report the synthesis and structure of the title compound, (I), (Fig. 1).

The molecular conformation is stabilised by an intramolecular O-H...N hydrogen bond (Table 1) and the dihedral angle between the aromatic ring planes is 79.55 (18)°. In the crystal, an intermolecular N-H...O hydrogen bond lead to [100] chains of molecules.

### Experimental

3 mmol of 2'-hydroxyacetophenone (3 mmol) was added to a solution of benzenesulfonyl hydrazide (3 mmol) in 10 ml of 95% ethanol. The mixture was continuously stirred for 3 h at refluxing temperature, evaporating some ethanol, then, upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 68%). Colourless blocks of (I) were obtained by evaporation from a methanol solution after 3 days.

### Refinement

The H atoms were placed geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å, N—H = 0.90 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

### Figures

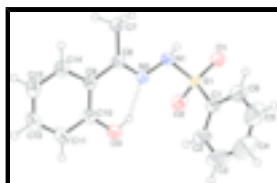


Fig. 1. The molecular structure of (I) showing 40% displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bond is indicated by a double-dashed line.

## *N'*-[1-(2-Hydroxyphenyl)ethylidene]benzenesulfonohydrazide

### Crystal data

$\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_3\text{S}$

$M_r = 290.33$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 5.2435$  (9) Å

$F_{000} = 608$

$D_x = 1.362$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2187 reflections

$\theta = 2.5$ – $26.2^\circ$

# supplementary materials

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$b = 13.2515 (18) \text{ \AA}$   
 $c = 20.375 (2) \text{ \AA}$   
 $\beta = 90.531 (2)^\circ$   
 $V = 1415.7 (3) \text{ \AA}^3$   
 $Z = 4$

$\mu = 0.24 \text{ mm}^{-1}$   
 $T = 298 (2) \text{ K}$   
Block, colourless  
 $0.50 \times 0.40 \times 0.37 \text{ mm}$

## Data collection

Bruker SMART CCD diffractometer  
Radiation source: fine-focus sealed tube  
Monochromator: graphite  
 $T = 298(2) \text{ K}$   
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.891, T_{\max} = 0.918$   
7165 measured reflections

2484 independent reflections  
1755 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$   
 $\theta_{\max} = 25.0^\circ$   
 $\theta_{\min} = 1.8^\circ$   
 $h = -6 \rightarrow 6$   
 $k = -15 \rightarrow 15$   
 $l = -20 \rightarrow 24$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.131$   
 $S = 1.04$   
2484 reflections  
182 parameters

Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.8643P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$   
Extinction correction: SHELXL97 (Sheldrick, 2008),  
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.018 (2)

Primary atom site location: structure-invariant direct methods  
Secondary atom site location: difference Fourier map

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.3921 (4)	0.13317 (15)	0.94596 (10)	0.0397 (6)
H1	0.5569	0.1345	0.9587	0.048*
N2	0.3516 (4)	0.21056 (16)	0.90070 (10)	0.0378 (5)
O1	0.2888 (4)	0.06000 (14)	1.05125 (9)	0.0589 (6)
O2	-0.0427 (4)	0.15363 (16)	0.98874 (10)	0.0560 (6)
O3	0.0643 (4)	0.35673 (15)	0.86405 (10)	0.0590 (6)
H3	0.1123	0.3112	0.8884	0.089*
S1	0.21361 (14)	0.14329 (5)	1.01133 (3)	0.0403 (3)
C1	0.2935 (5)	0.2560 (2)	1.05229 (13)	0.0414 (7)
C2	0.1465 (7)	0.3404 (2)	1.04223 (18)	0.0659 (10)
H2	0.0090	0.3388	1.0131	0.079*
C3	0.2063 (10)	0.4282 (3)	1.0763 (2)	0.0931 (14)
H3A	0.1108	0.4864	1.0694	0.112*
C4	0.4057 (10)	0.4288 (4)	1.1200 (3)	0.1013 (16)
H4	0.4428	0.4871	1.1436	0.122*
C5	0.5504 (8)	0.3446 (4)	1.1293 (2)	0.0922 (14)
H5	0.6876	0.3463	1.1586	0.111*
C6	0.4952 (6)	0.2567 (3)	1.09574 (17)	0.0651 (9)
H6	0.5928	0.1990	1.1024	0.078*
C7	0.6988 (6)	0.1407 (2)	0.83455 (14)	0.0472 (7)
H7A	0.8593	0.1693	0.8479	0.071*
H7B	0.7018	0.1265	0.7884	0.071*
H7C	0.6699	0.0793	0.8584	0.071*
C8	0.4892 (5)	0.21397 (19)	0.84856 (12)	0.0357 (6)
C9	0.4232 (5)	0.29502 (19)	0.80152 (12)	0.0381 (6)
C10	0.2176 (5)	0.3608 (2)	0.81077 (13)	0.0421 (7)
C11	0.1611 (6)	0.4351 (2)	0.76493 (15)	0.0553 (8)
H11	0.0230	0.4779	0.7716	0.066*
C12	0.3072 (7)	0.4462 (3)	0.70987 (16)	0.0619 (9)
H12	0.2675	0.4960	0.6793	0.074*
C13	0.5109 (7)	0.3840 (3)	0.70007 (15)	0.0631 (9)
H13	0.6118	0.3920	0.6631	0.076*
C14	0.5665 (6)	0.3096 (2)	0.74492 (14)	0.0524 (8)
H14	0.7047	0.2673	0.7373	0.063*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0424 (14)	0.0379 (12)	0.0388 (12)	0.0084 (10)	0.0018 (10)	0.0056 (10)
N2	0.0423 (13)	0.0336 (12)	0.0374 (12)	0.0046 (10)	-0.0001 (10)	0.0029 (10)
O1	0.0933 (17)	0.0375 (11)	0.0461 (12)	0.0088 (11)	0.0154 (11)	0.0074 (9)
O2	0.0413 (13)	0.0634 (14)	0.0636 (13)	-0.0068 (10)	0.0049 (10)	-0.0136 (11)
O3	0.0633 (15)	0.0536 (13)	0.0605 (13)	0.0217 (11)	0.0148 (11)	0.0146 (10)
S1	0.0473 (5)	0.0335 (4)	0.0402 (4)	0.0002 (3)	0.0065 (3)	-0.0006 (3)

## supplementary materials

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C1	0.0423 (17)	0.0383 (15)	0.0436 (16)	-0.0023 (12)	0.0051 (13)	-0.0047 (12)
C2	0.081 (3)	0.0445 (19)	0.073 (2)	0.0108 (17)	-0.0073 (19)	-0.0115 (16)
C3	0.123 (4)	0.046 (2)	0.111 (3)	0.009 (2)	0.011 (3)	-0.022 (2)
C4	0.102 (4)	0.084 (3)	0.118 (4)	-0.034 (3)	0.012 (3)	-0.050 (3)
C5	0.069 (3)	0.114 (4)	0.094 (3)	-0.019 (3)	-0.012 (2)	-0.045 (3)
C6	0.048 (2)	0.074 (2)	0.073 (2)	0.0026 (17)	-0.0069 (18)	-0.0137 (18)
C7	0.0505 (19)	0.0457 (16)	0.0457 (16)	0.0071 (14)	0.0069 (14)	-0.0027 (13)
C8	0.0362 (15)	0.0342 (14)	0.0366 (14)	-0.0051 (12)	-0.0013 (12)	-0.0055 (11)
C9	0.0418 (17)	0.0361 (14)	0.0363 (14)	-0.0049 (12)	-0.0048 (12)	-0.0004 (11)
C10	0.0421 (17)	0.0400 (15)	0.0442 (16)	-0.0037 (13)	-0.0021 (13)	0.0025 (13)
C11	0.056 (2)	0.0466 (18)	0.063 (2)	0.0022 (15)	-0.0082 (16)	0.0154 (15)
C12	0.071 (2)	0.059 (2)	0.055 (2)	-0.0072 (18)	-0.0139 (18)	0.0214 (16)
C13	0.076 (3)	0.069 (2)	0.0450 (18)	-0.0073 (19)	0.0049 (17)	0.0140 (16)
C14	0.056 (2)	0.0562 (19)	0.0448 (17)	0.0011 (15)	0.0025 (15)	0.0065 (14)

### *Geometric parameters (Å, °)*

N1—N2	1.394 (3)	C5—H5	0.9300
N1—S1	1.641 (2)	C6—H6	0.9300
N1—H1	0.9000	C7—C8	1.496 (4)
N2—C8	1.291 (3)	C7—H7A	0.9600
O1—S1	1.4246 (19)	C7—H7B	0.9600
O2—S1	1.423 (2)	C7—H7C	0.9600
O3—C10	1.358 (3)	C8—C9	1.478 (4)
O3—H3	0.8200	C9—C14	1.395 (4)
S1—C1	1.760 (3)	C9—C10	1.401 (4)
C1—C2	1.372 (4)	C10—C11	1.387 (4)
C1—C6	1.373 (4)	C11—C12	1.372 (4)
C2—C3	1.390 (5)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.366 (5)
C3—C4	1.367 (6)	C12—H12	0.9300
C3—H3A	0.9300	C13—C14	1.374 (4)
C4—C5	1.361 (6)	C13—H13	0.9300
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.380 (5)		
N2—N1—S1	113.09 (16)	C5—C6—H6	120.6
N2—N1—H1	108.5	C8—C7—H7A	109.5
S1—N1—H1	108.5	C8—C7—H7B	109.5
C8—N2—N1	119.2 (2)	H7A—C7—H7B	109.5
C10—O3—H3	109.5	C8—C7—H7C	109.5
O2—S1—O1	120.99 (14)	H7A—C7—H7C	109.5
O2—S1—N1	106.82 (12)	H7B—C7—H7C	109.5
O1—S1—N1	104.08 (11)	N2—C8—C9	115.5 (2)
O2—S1—C1	106.95 (13)	N2—C8—C7	123.5 (2)
O1—S1—C1	108.88 (13)	C9—C8—C7	121.0 (2)
N1—S1—C1	108.63 (12)	C14—C9—C10	116.5 (2)
C2—C1—C6	121.3 (3)	C14—C9—C8	120.8 (2)
C2—C1—S1	119.3 (2)	C10—C9—C8	122.7 (2)
C6—C1—S1	119.3 (2)	O3—C10—C11	116.3 (3)

C1—C2—C3	118.9 (4)	O3—C10—C9	123.0 (2)
C1—C2—H2	120.5	C11—C10—C9	120.7 (3)
C3—C2—H2	120.5	C12—C11—C10	120.6 (3)
C4—C3—C2	119.9 (4)	C12—C11—H11	119.7
C4—C3—H3A	120.1	C10—C11—H11	119.7
C2—C3—H3A	120.1	C13—C12—C11	119.9 (3)
C5—C4—C3	120.5 (4)	C13—C12—H12	120.1
C5—C4—H4	119.7	C11—C12—H12	120.1
C3—C4—H4	119.7	C12—C13—C14	119.8 (3)
C4—C5—C6	120.6 (4)	C12—C13—H13	120.1
C4—C5—H5	119.7	C14—C13—H13	120.1
C6—C5—H5	119.7	C13—C14—C9	122.4 (3)
C1—C6—C5	118.8 (4)	C13—C14—H14	118.8
C1—C6—H6	120.6	C9—C14—H14	118.8
S1—N1—N2—C8	176.68 (19)	N1—N2—C8—C9	176.6 (2)
N2—N1—S1—O2	52.5 (2)	N1—N2—C8—C7	-2.1 (4)
N2—N1—S1—O1	-178.43 (18)	N2—C8—C9—C14	176.8 (2)
N2—N1—S1—C1	-62.5 (2)	C7—C8—C9—C14	-4.5 (4)
O2—S1—C1—C2	-17.1 (3)	N2—C8—C9—C10	-3.1 (4)
O1—S1—C1—C2	-149.4 (3)	C7—C8—C9—C10	175.6 (3)
N1—S1—C1—C2	97.9 (3)	C14—C9—C10—O3	-178.9 (3)
O2—S1—C1—C6	160.2 (2)	C8—C9—C10—O3	1.0 (4)
O1—S1—C1—C6	27.9 (3)	C14—C9—C10—C11	0.8 (4)
N1—S1—C1—C6	-84.8 (3)	C8—C9—C10—C11	-179.3 (3)
C6—C1—C2—C3	0.8 (5)	O3—C10—C11—C12	179.1 (3)
S1—C1—C2—C3	178.0 (3)	C9—C10—C11—C12	-0.6 (5)
C1—C2—C3—C4	-1.3 (6)	C10—C11—C12—C13	-0.3 (5)
C2—C3—C4—C5	1.6 (7)	C11—C12—C13—C14	1.0 (5)
C3—C4—C5—C6	-1.3 (7)	C12—C13—C14—C9	-0.7 (5)
C2—C1—C6—C5	-0.5 (5)	C10—C9—C14—C13	-0.2 (4)
S1—C1—C6—C5	-177.7 (3)	C8—C9—C14—C13	180.0 (3)
C4—C5—C6—C1	0.7 (6)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3 $\cdots$ N2	0.82	1.85	2.561 (3)	145
N1—H1 $\cdots$ O2 <sup>i</sup>	0.90	2.20	3.093 (3)	174

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1

