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(*E*)-2-[(1,2,3-Thiadiazol-5-yl)iminomethyl]phenol

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In the title compound, $C_9H_7N_3OS$, the structure is stabilized by intramolecular O—H···N and intermolecular C—H···O and C—H···N hydrogen bonds. The intermolecular hydrogen bonds link the molecules into a three-dimensional supramolecular network.

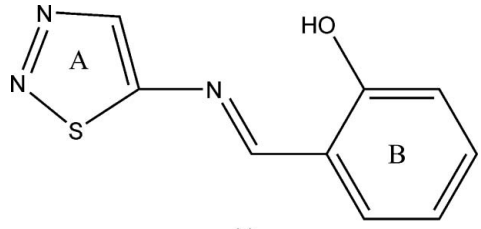
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.090
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I), with a number of reactive centers, could be an excellent candidate for the construction of supramolecular architectures.



(I)

In (I) the rings *A* and *B* are essentially coplanar, with a dihedral angle between the two rings of 1.17 (11)° (Fig. 1). The bonding about S1 is slightly asymmetrical (Table 1). The remaining bond lengths and angles of ring *A* are in agreement with values reported for similar structures (Capuano *et al.*, 1983).

The structure is stabilized by intramolecular and intermolecular hydrogen-bond interactions (Table 2). In the crystal structure, adjacent molecules are linked *via* intermolecular C1—H1···O1^{ii} interactions into a one-dimensional infinite chain. In addition, C3—H2···N2^{i} hydrogen bonds link these chains into a three dimensional supramolecular network (Fig. 2).

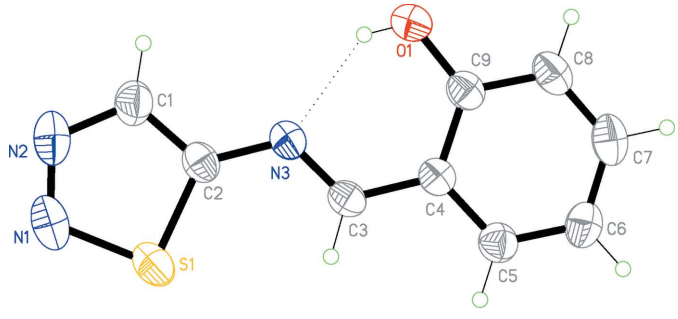


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. The dotted line indicates the intramolecular hydrogen bond.

Experimental

1,2,3-Thiadiazol-5-amine was prepared as described in the literature (Guo, 1998). 1,2,3-Thiadiazol-5-amine (10.1 g, 0.1 mol) and 2-hydroxybenzaldehyde (12.2 g, 0.1 mol) were dissolved in 30 ml of methanol. The mixture was stirred at room temperature for 24 h. The resulting yellow–orange precipitate was removed, washed with methanol and then dried *in vacuo*. Suitable single crystals were grown by slow evaporation from an ethanol solution (yield 75%,).

Crystal data

$C_9H_7N_3OS$
M_r = 205.25
Orthorhombic, $P2_12_12_1$
a = 4.7477 (9) Å
b = 11.415 (2) Å
c = 16.798 (3) Å
V = 910.4 (3) Å^3
Z = 4
D_x = 1.497 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 293 (2) K
Block, yellow
0.48 × 0.33 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.861, T_{max} = 0.934
8509 measured reflections
2054 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.090
S = 1.17
2054 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 808 Friedel pairs
Flack parameter: 0.01 (8)

Table 1
Selected geometric parameters (Å, °).

S1—N1	1.6950 (18)	N2—N1	1.286 (2)
S1—C2	1.7186 (16)	N2—C1	1.352 (2)
C2—C1	1.369 (3)		
N1—S1—C2	92.74 (8)	N1—N2—C1	114.55 (17)
C1—C2—N3	124.48 (15)	N2—C1—C2	115.25 (17)
C1—C2—S1	106.41 (12)	N2—N1—S1	111.05 (13)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H2···N2^{i}	0.93	2.67	3.533 (2)	155
C1—H1···O1^{ii}	0.93	2.43	3.241 (2)	146
O1—H7···N3	0.82	1.92	2.6408 (18)	146

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

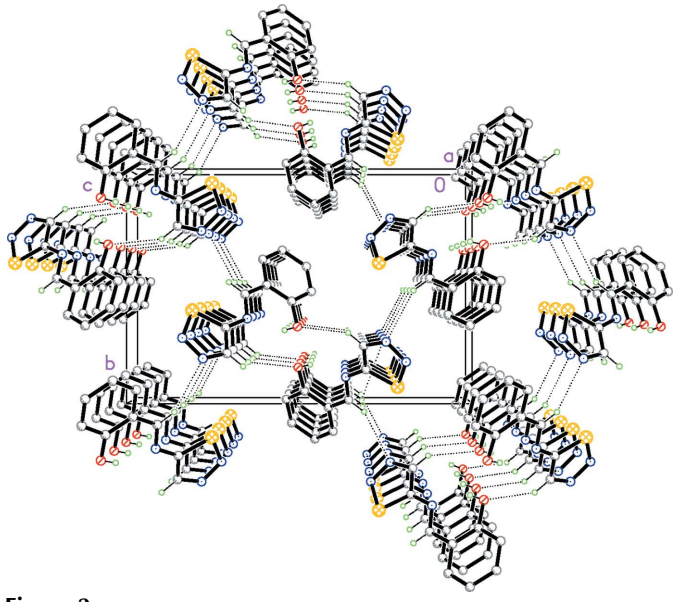


Figure 2
A partial packing view, showing the three-dimensional hydrogen-bonding network. Dotted lines indicate the hydrogen-bonded interactions. H atoms not involved in hydrogen bonds have been omitted for clarity.

All H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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