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A monoclinic modification of 2-[(1,3-benzothiazol-2-yl)iminomethyl]phenol

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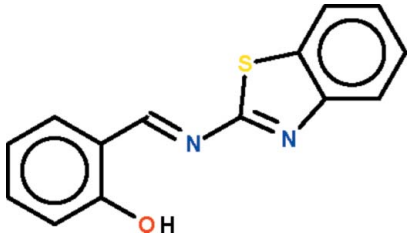
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 15.8.

In the title Schiff base, $C_{14}H_{10}N_2OS$, the azomethine double bond is in an E configuration; the benzothiazolyl ring (r.m.s. deviation = 0.007 Å) is coplanar with the phenylene ring (r.m.s. deviation = 0.007 Å), the two rings being slightly bent at 2.6 (1)°. The hydroxy H atom forms an intramolecular hydrogen bond to the imino group. The bond dimensions of the monoclinic modification are similar to those of the orthorhombic modification [Liu *et al.* (2009). *Acta Cryst.* E**65**, o738].

Related literature

For an orthorhombic modification of this structure, see: Liu *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{10}N_2OS$ M_r = 254.30
Monoclinic, Pn
a = 8.6391 (4) Å
b = 6.2313 (4) Å
c = 11.4459 (8) Å
β = 108.893 (1)°
V = 582.97 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 100 K
0.14 × 0.13 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.979
5307 measured reflections
2599 independent reflections
2512 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.05
2599 reflections
164 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1242 Friedel pairs
Flack parameter: 0.27 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.87	1.73	2.550 (2)	156

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdul Aziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2043).

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supporting information

Acta Cryst. (2010). E**66**, o1826 [doi:10.1107/S1600536810023755]

A monoclinic modification of 2-[(1,3-benzothiazol-2-yl)iminomethyl]phenol

Abdullah M. Asiri, Salman A. Khan, Kong Wai Tan and Seik Weng Ng

S1. Comment

The orthorhombic modification of 2-[(1,3-benzothiazol-2-yl)iminomethyl]phenol (Scheme I) is a flat molecule having a (calculated) density of 1.409 g ml^{-1} (Liu *et al.*, 2009). In the monoclinic modification, the packing is more compact (calculated density 1.449 g ml^{-1}). The benzisotholyl ring [r.m.s. deviation 0.007 Å] is co-planar with the phenylene ring [r.m.s. deviation 0.007 Å], the two rings being slightly bent by 2.6 (1) ° only. The hydroxy H-atom forms an intramolecular hydrogen bond to the imino group (Fig. 1). The r.m.s. deviation of the non-hydrogen atoms for the least-squares plane is 0.034 Å, and all deviations deviate by 0.002 Å only.

S2. Experimental

2-Aminobenzothiazole (0.50 g, 4.4 mol) and salicyladehyde (0.66 g, 4.4 mol) were heated in methanol (15 ml) for 5 h. Yellowish-orange crystals deposited when the solution was set aside for a day.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 Å, U(H) 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation. The hydroxy H-atom was located in a difference Fourier map, but attempts to refine it even with a distance restraint led to a small temperature factor. The position and temperature factor were not refined. The structure is a racemic twin, the explicit refinement of the Flack parameter from 1242 Friedel pairs gave a value of 0.27 (8).

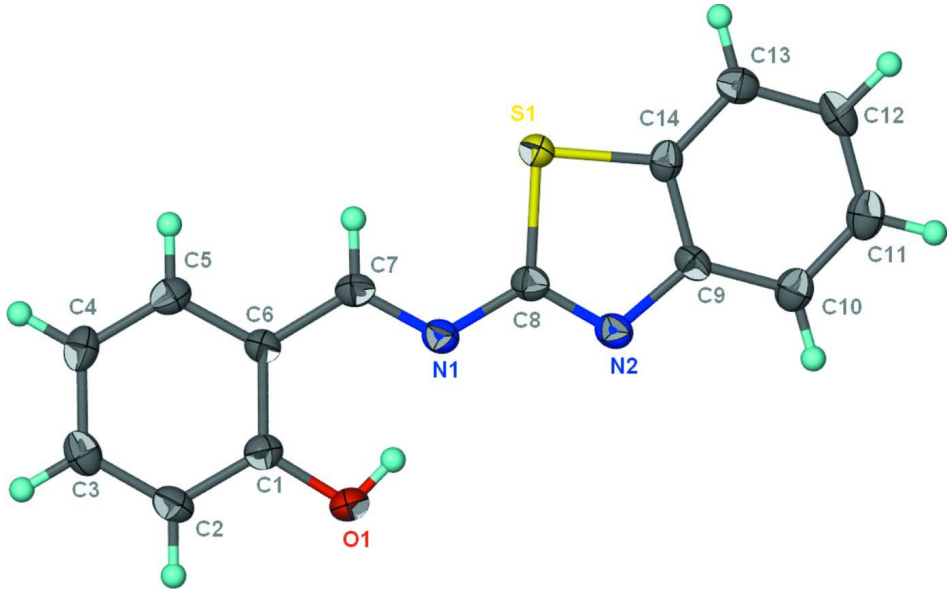

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{14}H_{10}N_2OS$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-[(1,3-benzothiazol-2-yl)iminomethyl]phenol

Crystal data

$C_{14}H_{10}N_2OS$
$M_r = 254.30$
Monoclinic, *Pn*
Hall symbol: P -2yac
$a = 8.6391$ (4) Å
$b = 6.2313$ (4) Å
$c = 11.4459$ (8) Å
$\beta = 108.893$ (1)°
$V = 582.97$ (6) Å^3
$Z = 2$
$F(000) = 264$
$D_x = 1.449$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3896 reflections
$\theta = 2.6$–$28.3°$
$\mu = 0.26$ mm^{-1}
$T = 100$ K
Prism, orange
0.14 × 0.13 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.964$, $T_{max} = 0.979$
5307 measured reflections
2599 independent reflections
2512 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$
$h = -11 \rightarrow 10$
$k = -8 \rightarrow 8$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.110$
$S = 1.05$
2599 reflections
164 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 0.0645P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Absolute structure: Flack (1983), 1242 Friedel pairs
Absolute structure parameter: 0.27 (8)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.50007 (6)	0.06429 (7)	0.49993 (5)	0.01864 (15)
O1	0.7048 (2)	0.5684 (3)	0.89741 (16)	0.0277 (4)
H1	0.6924	0.4623	0.8462	0.042*
N1	0.6095 (2)	0.3254 (3)	0.70823 (16)	0.0186 (4)
N2	0.7613 (2)	0.0261 (3)	0.69409 (17)	0.0193 (4)
C1	0.5700 (3)	0.6867 (4)	0.84466 (19)	0.0195 (4)
C2	0.5445 (3)	0.8696 (4)	0.9059 (2)	0.0222 (4)
H2	0.6227	0.9096	0.9825	0.027*
C3	0.4058 (3)	0.9936 (4)	0.8561 (2)	0.0226 (5)
H3	0.3895	1.1183	0.8985	0.027*
C4	0.2898 (3)	0.9363 (3)	0.7441 (2)	0.0228 (5)
H4	0.1937	1.0201	0.7108	0.027*
C5	0.3153 (3)	0.7571 (4)	0.68168 (19)	0.0214 (4)
H5	0.2366	0.7193	0.6049	0.026*
C6	0.4554 (3)	0.6303 (3)	0.72981 (19)	0.0175 (4)
C7	0.4806 (3)	0.4437 (3)	0.6638 (2)	0.0188 (4)
H7	0.4019	0.4071	0.5868	0.023*
C8	0.6349 (3)	0.1448 (3)	0.64566 (19)	0.0184 (4)
C9	0.7588 (3)	−0.1475 (3)	0.61665 (18)	0.0178 (4)
C10	0.8777 (3)	−0.3090 (4)	0.6428 (2)	0.0228 (4)
H10	0.9681	−0.3056	0.7170	0.027*
C11	0.8612 (3)	−0.4729 (4)	0.5589 (2)	0.0249 (5)
H11	0.9414	−0.5832	0.5757	0.030*
C12	0.7290 (3)	−0.4798 (4)	0.4498 (2)	0.0229 (5)
H12	0.7212	−0.5939	0.3931	0.027*
C13	0.6081 (3)	−0.3219 (4)	0.4225 (2)	0.0213 (4)
H13	0.5170	−0.3277	0.3488	0.026*
C14	0.6257 (3)	−0.1556 (3)	0.5070 (2)	0.0190 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0181 (2)	0.0172 (2)	0.0187 (2)	−0.0003 (2)	0.00322 (17)	−0.00262 (19)
O1	0.0216 (9)	0.0314 (10)	0.0232 (9)	0.0063 (7)	−0.0024 (7)	−0.0064 (6)
N1	0.0193 (8)	0.0166 (8)	0.0183 (8)	−0.0016 (7)	0.0040 (7)	−0.0015 (7)
N2	0.0222 (10)	0.0148 (8)	0.0191 (9)	−0.0020 (7)	0.0042 (7)	−0.0008 (7)
C1	0.0181 (10)	0.0220 (10)	0.0181 (9)	−0.0008 (8)	0.0051 (8)	−0.0004 (8)
C2	0.0235 (11)	0.0215 (10)	0.0211 (10)	−0.0032 (9)	0.0066 (9)	−0.0052 (8)
C3	0.0265 (12)	0.0193 (10)	0.0263 (11)	−0.0017 (9)	0.0144 (9)	−0.0023 (8)

C4	0.0228 (12)	0.0211 (11)	0.0255 (11)	0.0054 (8)	0.0095 (9)	0.0051 (8)
C5	0.0197 (10)	0.0245 (10)	0.0190 (9)	0.0002 (9)	0.0048 (8)	0.0025 (8)
C6	0.0179 (10)	0.0178 (9)	0.0164 (9)	−0.0011 (8)	0.0050 (8)	−0.0012 (8)
C7	0.0173 (10)	0.0200 (11)	0.0177 (10)	−0.0029 (8)	0.0035 (8)	−0.0002 (7)
C8	0.0196 (10)	0.0168 (10)	0.0182 (9)	−0.0025 (8)	0.0051 (8)	0.0001 (7)
C9	0.0221 (10)	0.0148 (9)	0.0175 (9)	−0.0025 (8)	0.0077 (8)	−0.0021 (8)
C10	0.0228 (11)	0.0209 (10)	0.0249 (10)	0.0016 (9)	0.0081 (8)	0.0032 (8)
C11	0.0245 (12)	0.0224 (11)	0.0311 (12)	0.0032 (9)	0.0136 (10)	0.0047 (9)
C12	0.0282 (13)	0.0182 (10)	0.0276 (12)	−0.0036 (9)	0.0166 (10)	−0.0058 (9)
C13	0.0205 (10)	0.0224 (11)	0.0208 (10)	−0.0043 (9)	0.0063 (8)	−0.0018 (8)
C14	0.0178 (10)	0.0156 (9)	0.0249 (10)	0.0012 (8)	0.0088 (8)	0.0022 (8)

Geometric parameters (Å, º)

S1—C14	1.733 (2)	C4—H4	0.9500
S1—C8	1.770 (2)	C5—C6	1.400 (3)
O1—C1	1.345 (3)	C5—H5	0.9500
O1—H1	0.8672	C6—C7	1.442 (3)
N1—C7	1.294 (3)	C7—H7	0.9500
N1—C8	1.389 (3)	C9—C10	1.399 (3)
N2—C8	1.286 (3)	C9—C14	1.402 (3)
N2—C9	1.394 (3)	C10—C11	1.378 (3)
C1—C2	1.393 (3)	C10—H10	0.9500
C1—C6	1.410 (3)	C11—C12	1.393 (4)
C2—C3	1.383 (4)	C11—H11	0.9500
C2—H2	0.9500	C12—C13	1.395 (3)
C3—C4	1.394 (4)	C12—H12	0.9500
C3—H3	0.9500	C13—C14	1.392 (3)
C4—C5	1.381 (3)	C13—H13	0.9500
C14—S1—C8	88.21 (11)	N1—C7—H7	119.7
C1—O1—H1	102.4	C6—C7—H7	119.7
C7—N1—C8	121.20 (18)	N2—C8—N1	119.83 (19)
C8—N2—C9	109.65 (18)	N2—C8—S1	116.81 (16)
O1—C1—C2	118.56 (19)	N1—C8—S1	123.36 (17)
O1—C1—C6	121.8 (2)	N2—C9—C10	124.3 (2)
C2—C1—C6	119.7 (2)	N2—C9—C14	115.84 (19)
C3—C2—C1	120.4 (2)	C10—C9—C14	119.9 (2)
C3—C2—H2	119.8	C11—C10—C9	118.8 (2)
C1—C2—H2	119.8	C11—C10—H10	120.6
C2—C3—C4	120.3 (2)	C9—C10—H10	120.6
C2—C3—H3	119.8	C10—C11—C12	121.1 (2)
C4—C3—H3	119.8	C10—C11—H11	119.4
C5—C4—C3	119.7 (2)	C12—C11—H11	119.4
C5—C4—H4	120.2	C13—C12—C11	121.1 (2)
C3—C4—H4	120.2	C13—C12—H12	119.5
C4—C5—C6	121.0 (2)	C11—C12—H12	119.5
C4—C5—H5	119.5	C14—C13—C12	117.7 (2)

C6—C5—H5	119.5	C14—C13—H13	121.2
C5—C6—C1	118.87 (19)	C12—C13—H13	121.2
C5—C6—C7	120.47 (19)	C13—C14—C9	121.5 (2)
C1—C6—C7	120.7 (2)	C13—C14—S1	129.07 (18)
N1—C7—C6	120.7 (2)	C9—C14—S1	109.47 (16)
O1—C1—C2—C3	−178.7 (2)	C14—S1—C8—N2	1.30 (18)
C6—C1—C2—C3	1.4 (3)	C14—S1—C8—N1	−178.28 (18)
C1—C2—C3—C4	0.2 (4)	C8—N2—C9—C10	−179.1 (2)
C2—C3—C4—C5	−1.2 (4)	C8—N2—C9—C14	0.2 (3)
C3—C4—C5—C6	0.6 (3)	N2—C9—C10—C11	179.7 (2)
C4—C5—C6—C1	0.9 (3)	C14—C9—C10—C11	0.4 (3)
C4—C5—C6—C7	−180.0 (2)	C9—C10—C11—C12	−0.1 (3)
O1—C1—C6—C5	178.2 (2)	C10—C11—C12—C13	−0.6 (4)
C2—C1—C6—C5	−1.9 (3)	C11—C12—C13—C14	1.1 (3)
O1—C1—C6—C7	−0.9 (3)	C12—C13—C14—C9	−0.8 (3)
C2—C1—C6—C7	179.0 (2)	C12—C13—C14—S1	179.15 (17)
C8—N1—C7—C6	179.8 (2)	N2—C9—C14—C13	−179.33 (19)
C5—C6—C7—N1	−179.6 (2)	C10—C9—C14—C13	0.0 (3)
C1—C6—C7—N1	−0.5 (3)	N2—C9—C14—S1	0.7 (2)
C9—N2—C8—N1	178.51 (18)	C10—C9—C14—S1	−179.89 (17)
C9—N2—C8—S1	−1.1 (2)	C8—S1—C14—C13	179.0 (2)
C7—N1—C8—N2	−177.6 (2)	C8—S1—C14—C9	−1.04 (16)
C7—N1—C8—S1	2.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.87	1.73	2.550 (2)	156