Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2-[(4-Hydroxyphenyl)iminomethyl]-thiophene

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Received 27 January 2000
Accepted 26 May 2000

The molecular structure of the title compound, $C_{11}H_9NOS$, has three planar moieties, two of which are rings, namely the hydroxyphenyl and the thiophene, with an angle of 20.76 (10)° between them. The crystal structure is stabilized by an O—H···N hydrogen bond and by C—H···O intermolecular interactions. The C···O intermolecular contact distance is 3.443 (2) Å.

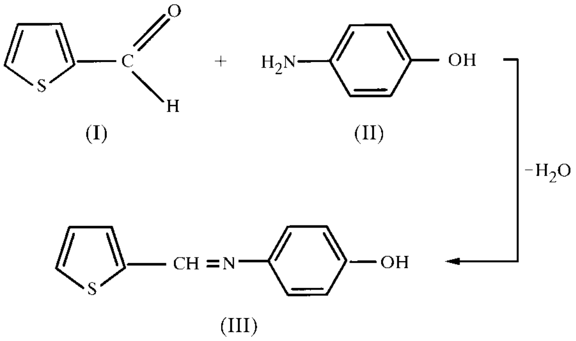
Comment

Most Schiff bases possess antibacterial, anticancer, anti-inflammatory and antitoxic activities (Williams, 1972), and the sulfur-containing Schiff bases are particularly effective. Schiff bases have been used extensively as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1978). The intramolecular hydrogen bond between the O and N atoms plays an important role in the formation of metal complexes and Schiff base compounds in the solid state *via* proton transfer from the hydroxy-O atom to the imine-N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). Charge transport occurs through overlapping intramolecular π orbitals with proton transfer (Xu *et al.*, 1994). In this paper, we report the structure of 2-[(4-hydroxyphenyl)iminomethyl]thiophene, (III).

An *ORTEP*III (Burnett & Johnson, 1996) plot of compound (III) is shown in Fig. 1. The C7═N1 bond length of 1.282 (2) Å is typical of a double bond, which is similar to the corresponding bond lengths in *N*-(2,4-dinitrophenyl)-*N*-methylhydrazone [1.279 (2) Å; Aygün *et al.*, 1998], 2-salicylideneamino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carbonitrile [1.281 (2) Å; Elerman & Elmalı, 1998] and 4-ethyl-2-(2-hydroxynapthylmethylidene)amino-5-methyl-3-thiophene carbonitrile [1.293 (3) Å; Elerman *et al.*, 1997].

The O1—C4 and N1—C1 bond distances are 1.358 (2) and 1.422 (2) Å, respectively, which are similar to the corresponding bond lengths in 4-ethyl-2-(2-hydroxynapthyl methylidene)amino-5-methyl-3-thiophene carbonitrile [1.357 (3) and 1.379 (4) Å, respectively; Elerman *et al.*, 1997], *N*-(5-bromosalicylidene)-2-aminopyridine [1.348 (6) and 1.414 (6) Å, respectively; Moustakali-Mavridis *et al.*, 1978] and 2,2′-azinodimethyldiphenol [1.364 (8) and 1.386 (9) Å, respectively; Xu *et al.*, 1994]. The increase in the electron density of the aromatic ring due to the –OH electron donor side group has made the N1—C1 bond distance in (III) longer than the values given by Elerman *et al.* (1997) and Xu *et al.* (1994). Other relevant bond lengths and angles are listed in Table 1.

The molecule of (III) is not planar. The dihedral angle between the planes of the hydroxyphenyl and thiophene rings is 20.76 (10)°, and these two planes make angles of 26.4 (2) and 5.8 (2)°, respectively, with the plane of the central moiety (C1—N1—C7—C8). The hydroxy-O atom deviates by 0.016 (1) Å from the plane of the phenyl ring.



The crystal structure of (III) is stabilized by an O—H···N hydrogen bond and by C—H···O intermolecular interactions. The O1···N1^{i}, N1^{i}···H1 and O1—H1 bond distances are 2.770 (2), 1.89 (3) and 0.89 (3) Å, respectively, and the O1—H1···N1^{i} angle is 169 (3)°. The C6···O1^{ii}, O1^{ii}···H6 and C6—H6 bond distances are 3.443 (2), 2.50 (2) and 0.96 (2) Å, respectively, and the C6—H6···O1^{ii} angle is 166 (2)° [symmetry codes: (i) $x + \frac{1}{2}, \frac{3}{2} - y, z + \frac{1}{2}$; (ii) $x + \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$]. The S···N distance is 3.135 (2) Å, which is shorter than the sum of the van der Waals radii (3.35 Å; Bondi, 1964).

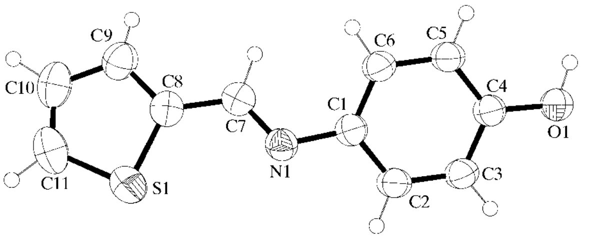


Figure 1
An *ORTEP*III (Burnett & Johnson, 1996) drawing of compound (III) showing the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small spheres of arbitrary size.

Experimental

Compound (III) was prepared *via* the reaction of 2-thiophenecarbaldehyde, (I), with 4-aminophenol, (II), by modifying the methods of Kamonuah (1992) and Rao *et al.* (1985). The Schiff base crystallized out on cooling the hot reaction mixture and was recrystallized from ethanol several times for purification. Crystals of (III) suitable for X-ray diffraction were obtained by slow cooling to room temperature of a saturated solution in hot tetrahydrofuran–chloroform (2:1).

Crystal data

$C_{11}H_9NOS$
$M_r = 203.25$
Monoclinic, $P2_1/n$
$a = 6.4268\ (3)$ Å
$b = 14.3420\ (12)$ Å
$c = 10.7559\ (6)$ Å
$\beta = 90.618\ (4)°$
$V = 991.35\ (11)$ Å^3
$Z = 4$
$D_x = 1.362$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10.6–21.7°$
$\mu = 2.60$ mm^{-1}
$T = 293\ (2)$ K
Prismatic, light brown
0.48 × 0.42 × 0.24 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
$T_{\min} = 0.417$, $T_{\max} = 0.536$
2007 measured reflections
2007 independent reflections
1883 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 74.22°$
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 17$
$l = -13 \rightarrow 13$
3 standard reflections
frequency: 120 min
intensity decay: 1.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.125$
$S = 1.051$
2007 reflections
164 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.431P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0159 (13)

Table 1
Selected geometric parameters (Å, °).

S1—C11	1.705 (3)	C7—C8	1.447 (3)
S1—C8	1.712 (2)	C8—C9	1.369 (3)
O1—C4	1.358 (2)	C9—C10	1.400 (3)
N1—C7	1.282 (2)	C10—C11	1.336 (4)
N1—C1	1.422 (2)		
C11—S1—C8	91.58 (12)	O1—C4—C5	123.21 (16)
C7—N1—C1	119.69 (16)	O1—C4—C3	117.72 (16)
N1—C7—C8	123.52 (18)	C9—C8—S1	110.36 (16)
C6—C1—N1	124.37 (16)	C10—C11—S1	112.41 (19)

The H atoms were located from difference maps and refined isotropically. The C—H bond distances range from 0.90 (3) to 1.01 (3) Å, while $U_{\rm iso}$ values for the H atoms are in the range 0.051 (5)–0.098 (10) Å^2.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

The authors wish to acknowledge the use of the CAD-4 diffractometer (purchased under grant DPT/TBAG1 of the Scientific and Technical Research Council of Turkey) of the Department of Physics Engineering, Hacettepe University, Turkey.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1266). Services for accessing these data are described at the back of the journal.

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