Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-Methyl-2-[3-(trifluoromethyl)-phenyliminomethyl]phenol

Zarife Sibel Gül,[a] Ferda Erşahin,[b] Erbil Ağar[b] and Şamil Işık[a]*

[a]Department of Physics, Ondokuz Mayıs University, 55139 Samsun, Turkey, and [b]Department of Chemistry, Arts and Sciences Faculty, Ondokuz Mayıs University, 55139 Samsun, Turkey
Correspondence e-mail: sgul@omu.edu.tr

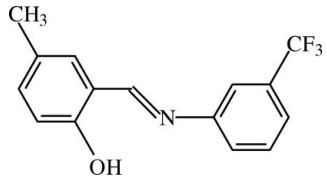
Received 9 April 2007; accepted 9 April 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.144; data-to-parameter ratio = 15.3.

The molecule of the title compound, $C_{15}H_{12}F_3NO$, is not planar and the dihedral angle between the planes of the two aromatic rings is 33.82 (11)°. The molecule exists in the phenol–imine tautomeric form, with a strong intramolecular O—H···N hydrogen bond [N···O = 2.609 (3) Å].

Related literature

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987). For related literature, see: Bernstein *et al.* (1995); Calligaris *et al.* (1972); Dey *et al.* (2001); Hökelek *et al.* (2000); Işik *et al.* (1998); Karadayı *et al.* (2003); Şahin *et al.* (2005); Xu *et al.* (1994).



Experimental

Crystal data

$C_{15}H_{12}F_3NO$
M_r = 279.26
Monoclinic, $P2_1/c$
a = 16.617 (2) Å
b = 4.7788 (4) Å
c = 21.169 (3) Å
β = 128.964 (9)°
V = 1307.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 K
0.80 × 0.24 × 0.14 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.933, T_{max} = 0.986
11701 measured reflections
2847 independent reflections
1178 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.144
S = 0.83
2847 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.78 (3)	1.89 (4)	2.609 (3)	153 (3)

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2361).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Calligaris, M., Nardin, G. & Randaccio, L. (1972). *Coord. Chem. Rev.* **7**, 385–403.
Cohen, M. D., Schmidt, G. M. J. & Flavian, S. (1964). *J. Chem. Soc.* pp. 2041–2051.
Dey, D. K., Dey, S. P., Elmalı, A. & Elerman, Y. (2001). *J. Mol. Struct.* **562**, 177–184.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hadjoudis, E., Vitterakis, M., Moustakali, I. & Mavridis, I. (1987). *Tetrahedron*, **43**, 1345–1360.
Hökelek, T., Kılıç, S., Işıklan, M. & Toy, M. (2000). *J. Mol. Struct.* **523**, 61–69.
Işik, Ş., Aygün, M., Kocaokutgen, H., Tahir, M. N., Büyükgüngör, O. & Erdönmez, A. (1998). *Acta Cryst.* C**54**, 859–860.
Karadayı, N., Gözüyeşil, S., Güzel, B. & Büyükgüngör, O. (2003). *Acta Cryst.* E**59**, o161–o163.
Şahin, O., Büyükgüngör, O., Albayrak, C. & Odabaşoğlu, M. (2005). *Acta Cryst.* E**61**, o1288–o1290.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-RED32* and *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Xu, X.-X., You, X.-Z., Sun, Z.-F., Wang, X. & Liu, H.-X. (1994). *Acta Cryst.* C**50**, 1169–1171.

  doi:10.1107/S1600536807017655

supplementary materials

Acta Cryst. (2007). E**63**, o2854 [**doi:10.1107/S1600536807017655**]

(*E*)-4-Methyl-2-[3-(trifluoromethyl)phenyliminomethyl]phenol

Z. S. Gül, F. Ersahin, E. Agar and S. Isik

Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). There are two characteristic properties of Schiff bases, viz. photochromism and thermochromism (Cohen *et al.*, 1964). These properties result from proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987). Schiff bases display two possible tautomeric forms, namely the phenol-imine and keto-amine forms. In the solid state, the keto-amine tautomer has been found in naphthaldimine (Hökelek *et al.*, 2000). However, in the solid state, it has been established that there is keto-amine tautomerism in naphthaldimine, while the phenol-imine form exists in salicylaldimine Schiff bases (Dey *et al.*, 2001).

Our investigations show that compound (I) adopts the phenol-imine tautomeric form. An ORTEP-3 (Farrugia, 1997) plot of the molecule of (I) is shown in Fig.1. The C8—N1 and C1—C7 bond lengths are 1.426 (3) and 1.450 (3) Å, respectively (Table 1), and agree with the corresponding distances in (*E*)-2-methoxy-6-[(2-trifluoromethylphenylimino)methyl]phenol [1.418 (5) and 1.454 (5) Å;Şahin *et al.*, 2005]. The N1═C7 bond length of 1.270 (3) Å is typical of a double bond, similar to the corresponding bond length in *N*-[3,5-bis(trifluoromethyl)phenyl]salicylaldimine [1.276 (4) Å; Karadayı *et al.*, 2003]. The O1—C6 distance of 1.352 (3) Å is close to the value of 1.349 (6) Å in 3-tert-butyl-2-hydroxy-5-methoxyazobenzene (Işik *et al.*, 1998). The dihedral angle between the C1—C6 and C8—C13 benzene rings is 33.82 (11)°.

There is a strong intramolecular hydrogen bond, O1—H1···N1, which forms an S(6) motif (Bernstein *et al.*, 1995). The O1···N1 distance of 2.609 (3) Å is comparable to those observed for analogous hydrogen bonds in *N*-[3,5-bis(trifluoromethyl)phenyl]salicylaldimine [2.604 (4) Å; Karadayı *et al.*, 2003] and 2,2-salicylaldimine [2.611 (6) Å; Xu *et al.*, 1994].

The crystal packing is stabilized by van der Waals interactions.

Experimental

The title compound was prepared by refluxing a mixture of a solution containing 5-methylsalicylaldehyde (0.1116 g, 0.82 mmol) in ethanol (20 ml) and a solution containing 3-trifluoromethylaniline (0.1 ml, 0.82 mmol) in ethanol (20 ml). The reaction mixture was stirred for 1 h under reflux. Crystals of (I) suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield 98% ; m.p. 342-344 K).

Refinement

The hydroxyl H atom was located in a difference map and refined isotropically. All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

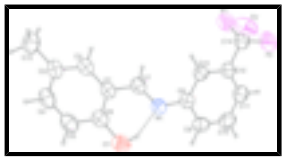


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. The dashed line indicates a hydrogen bond.

(*E*)-4-Methyl-2-[3-(trifluoromethyl)phenyliminomethyl]phenol

Crystal data

$C_{15}H_{12}F_3NO$	$F_{000} = 576$
$M_r = 279.26$	$D_x = 1.419$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 9332 reflections
$a = 16.617$ (2) Å	$\theta = 1.6$–29.4º
$b = 4.7788$ (4) Å	$\mu = 0.12$ mm^{-1}
$c = 21.169$ (3) Å	$T = 296$ K
$\beta = 128.964$ (9)º	Prism, yellow
$V = 1307.0$ (3) Å^3	0.80 × 0.24 × 0.14 mm
$Z = 4$	

Data collection

Stoe IPDSII diffractometer	2847 independent reflections
Radiation source: fine-focus sealed tube	1178 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.086$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 27.0$º
$T = 296$ K	$\theta_{min} = 1.6$º
ω scans	$h = -21 \rightarrow 21$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$k = -6 \rightarrow 5$
$T_{min} = 0.933$, $T_{max} = 0.986$	$l = -26 \rightarrow 26$
11701 measured reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.144$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
$S = 0.83$	$\Delta\rho_{min} = -0.16$ e Å^{-3}

2847 reflections
186 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.21905 (19)	1.2208 (5)	0.24517 (15)	0.0656 (6)
C2	0.2946 (2)	1.4021 (5)	0.30512 (16)	0.0729 (7)
H2	0.3560	1.4202	0.3129	0.087*
C3	0.2820 (2)	1.5566 (5)	0.35362 (15)	0.0745 (7)
C4	0.1880 (2)	1.5241 (6)	0.33849 (17)	0.0845 (8)
H4	0.1763	1.6269	0.3694	0.101*
C5	0.1121 (2)	1.3478 (7)	0.28030 (19)	0.0860 (8)
H5	0.0510	1.3293	0.2730	0.103*
C6	0.1262 (2)	1.1969 (6)	0.23220 (16)	0.0717 (7)
C7	0.2370 (2)	1.0634 (5)	0.19651 (16)	0.0692 (6)
H7	0.3005	1.0811	0.2075	0.083*
C8	0.19094 (19)	0.7413 (5)	0.09500 (14)	0.0657 (6)
C9	0.1082 (2)	0.6765 (6)	0.01500 (16)	0.0818 (8)
H9	0.0424	0.7425	−0.0078	0.098*
C10	0.1231 (2)	0.5146 (6)	−0.03081 (16)	0.0915 (9)
H10	0.0675	0.4745	−0.0846	0.110*
C11	0.2191 (2)	0.4130 (6)	0.00244 (16)	0.0832 (8)
H11	0.2286	0.3012	−0.0283	0.100*
C12	0.30132 (19)	0.4762 (5)	0.08130 (14)	0.0672 (6)
C13	0.28763 (19)	0.6390 (5)	0.12808 (14)	0.0656 (6)
H13	0.3437	0.6791	0.1818	0.079*
C14	0.4051 (2)	0.3679 (6)	0.11797 (17)	0.0799 (7)
C15	0.3651 (3)	1.7462 (6)	0.41932 (17)	0.0982 (9)
H15A	0.4137	1.7859	0.4102	0.147*
H15B	0.4002	1.6565	0.4711	0.147*
H15C	0.3346	1.9178	0.4187	0.147*

F1	0.47297 (14)	0.5629 (4)	0.13755 (14)	0.1293 (7)
F2	0.44860 (14)	0.2318 (4)	0.18725 (12)	0.1262 (7)
F3	0.40792 (15)	0.1895 (5)	0.07209 (13)	0.1483 (9)
N1	0.16910 (16)	0.9023 (4)	0.13934 (13)	0.0714 (6)
O1	0.04908 (16)	1.0249 (5)	0.17525 (14)	0.0905 (6)
H1	0.070 (3)	0.954 (7)	0.155 (2)	0.113 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0778 (16)	0.0658 (16)	0.0710 (15)	0.0124 (13)	0.0554 (14)	0.0147 (13)
C2	0.0826 (17)	0.0692 (16)	0.0824 (17)	0.0096 (14)	0.0593 (15)	0.0115 (14)
C3	0.102 (2)	0.0659 (15)	0.0740 (16)	0.0138 (15)	0.0639 (16)	0.0131 (13)
C4	0.114 (2)	0.084 (2)	0.0850 (18)	0.0252 (18)	0.0764 (18)	0.0172 (16)
C5	0.0942 (19)	0.099 (2)	0.0937 (19)	0.0155 (17)	0.0730 (18)	0.0133 (17)
C6	0.0779 (17)	0.0795 (18)	0.0718 (16)	0.0111 (15)	0.0538 (15)	0.0143 (14)
C7	0.0779 (16)	0.0710 (16)	0.0796 (17)	0.0051 (14)	0.0595 (15)	0.0097 (14)
C8	0.0737 (16)	0.0692 (15)	0.0634 (14)	−0.0013 (13)	0.0476 (13)	0.0042 (12)
C9	0.0714 (16)	0.097 (2)	0.0720 (17)	−0.0002 (14)	0.0424 (14)	0.0054 (15)
C10	0.089 (2)	0.112 (2)	0.0629 (16)	−0.0087 (18)	0.0425 (15)	−0.0117 (16)
C11	0.099 (2)	0.0899 (19)	0.0716 (17)	−0.0038 (17)	0.0593 (17)	−0.0080 (15)
C12	0.0777 (16)	0.0696 (16)	0.0649 (15)	0.0007 (13)	0.0499 (14)	0.0008 (12)
C13	0.0704 (15)	0.0716 (15)	0.0559 (13)	−0.0003 (12)	0.0402 (12)	0.0003 (12)
C14	0.092 (2)	0.0848 (19)	0.0755 (18)	−0.0003 (17)	0.0588 (16)	−0.0059 (16)
C15	0.130 (2)	0.090 (2)	0.0868 (19)	0.0026 (19)	0.0744 (19)	0.0024 (17)
F1	0.0990 (12)	0.1148 (14)	0.191 (2)	−0.0009 (11)	0.0992 (14)	0.0015 (14)
F2	0.1061 (13)	0.1614 (17)	0.1163 (14)	0.0445 (12)	0.0724 (11)	0.0485 (13)
F3	0.1314 (16)	0.176 (2)	0.1316 (16)	0.0307 (13)	0.0798 (14)	−0.0485 (15)
N1	0.0772 (13)	0.0758 (14)	0.0733 (13)	0.0040 (12)	0.0532 (12)	0.0067 (12)
O1	0.0824 (13)	0.1164 (17)	0.0894 (13)	0.0037 (12)	0.0621 (12)	0.0019 (12)

Geometric parameters (Å, °)

C1—C2	1.390 (3)	C9—C10	1.379 (4)
C1—C6	1.392 (3)	C9—H9	0.93
C1—C7	1.450 (3)	C10—C11	1.365 (4)
C2—C3	1.383 (3)	C10—H10	0.93
C2—H2	0.93	C11—C12	1.370 (3)
C3—C4	1.393 (4)	C11—H11	0.93
C3—C15	1.499 (4)	C12—C13	1.386 (3)
C4—C5	1.365 (4)	C12—C14	1.470 (4)
C4—H4	0.93	C13—H13	0.93
C5—C6	1.383 (4)	C14—F1	1.313 (3)
C5—H5	0.93	C14—F3	1.315 (3)
C6—O1	1.352 (3)	C14—F2	1.328 (3)
C7—N1	1.270 (3)	C15—H15A	0.96
C7—H7	0.93	C15—H15B	0.96
C8—C13	1.377 (3)	C15—H15C	0.96
C8—C9	1.388 (3)	O1—H1	0.78 (3)

C8—N1	1.426 (3)		
C2—C1—C6	118.9 (2)	C11—C10—C9	120.3 (3)
C2—C1—C7	120.1 (2)	C11—C10—H10	119.8
C6—C1—C7	121.0 (2)	C9—C10—H10	119.8
C3—C2—C1	122.6 (2)	C10—C11—C12	119.8 (3)
C3—C2—H2	118.7	C10—C11—H11	120.1
C1—C2—H2	118.7	C12—C11—H11	120.1
C2—C3—C4	116.2 (3)	C11—C12—C13	120.5 (2)
C2—C3—C15	122.0 (3)	C11—C12—C14	120.4 (2)
C4—C3—C15	121.8 (3)	C13—C12—C14	119.0 (2)
C5—C4—C3	122.9 (3)	C8—C13—C12	119.9 (2)
C5—C4—H4	118.6	C8—C13—H13	120.0
C3—C4—H4	118.6	C12—C13—H13	120.0
C4—C5—C6	119.9 (3)	F1—C14—F3	105.7 (2)
C4—C5—H5	120.1	F1—C14—F2	103.6 (2)
C6—C5—H5	120.1	F3—C14—F2	104.5 (2)
O1—C6—C5	118.0 (3)	F1—C14—C12	114.0 (2)
O1—C6—C1	122.5 (2)	F3—C14—C12	114.4 (2)
C5—C6—C1	119.5 (3)	F2—C14—C12	113.5 (2)
N1—C7—C1	122.4 (2)	C3—C15—H15A	109.5
N1—C7—H7	118.8	C3—C15—H15B	109.5
C1—C7—H7	118.8	H15A—C15—H15B	109.5
C13—C8—C9	119.0 (2)	C3—C15—H15C	109.5
C13—C8—N1	123.7 (2)	H15A—C15—H15C	109.5
C9—C8—N1	117.2 (2)	H15B—C15—H15C	109.5
C10—C9—C8	120.3 (3)	C7—N1—C8	120.9 (2)
C10—C9—H9	119.8	C6—O1—H1	105 (3)
C8—C9—H9	119.8		
C6—C1—C2—C3	1.2 (3)	C8—C9—C10—C11	1.0 (4)
C7—C1—C2—C3	−179.7 (2)	C9—C10—C11—C12	−1.1 (4)
C1—C2—C3—C4	−0.8 (3)	C10—C11—C12—C13	1.0 (4)
C1—C2—C3—C15	178.5 (2)	C10—C11—C12—C14	179.9 (3)
C2—C3—C4—C5	1.0 (4)	C9—C8—C13—C12	0.7 (3)
C15—C3—C4—C5	−178.4 (3)	N1—C8—C13—C12	177.8 (2)
C3—C4—C5—C6	−1.4 (4)	C11—C12—C13—C8	−0.8 (4)
C4—C5—C6—O1	−180.0 (2)	C14—C12—C13—C8	−179.7 (2)
C4—C5—C6—C1	1.7 (4)	C11—C12—C14—F1	115.3 (3)
C2—C1—C6—O1	−179.8 (2)	C13—C12—C14—F1	−65.9 (3)
C7—C1—C6—O1	1.1 (4)	C11—C12—C14—F3	−6.5 (4)
C2—C1—C6—C5	−1.6 (3)	C13—C12—C14—F3	172.3 (2)
C7—C1—C6—C5	179.3 (2)	C11—C12—C14—F2	−126.4 (3)
C2—C1—C7—N1	−177.7 (2)	C13—C12—C14—F2	52.5 (3)
C6—C1—C7—N1	1.4 (4)	C1—C7—N1—C8	−177.3 (2)
C13—C8—C9—C10	−0.8 (4)	C13—C8—N1—C7	31.7 (3)
N1—C8—C9—C10	−178.1 (2)	C9—C8—N1—C7	−151.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O1—H1···N1	0.78 (3)	1.89 (4)	2.609 (3)	153 (3)

Fig. 1