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(*E*)-2-Methyl-6-[3-(trifluoromethyl)-phenyliminomethyl]phenol

Abdullah Akkaya,[a]* Ferda Erşahin,[b] Erbil Ağar,[b] İsmet Şenel[a] and Orhan Büyükgüngör[a]

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

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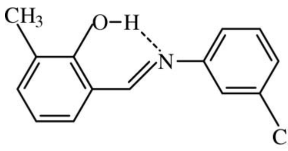
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.076; wR factor = 0.257; data-to-parameter ratio = 9.9.

The title compound, $C_{15}H_{12}NOF_3$, adopts the phenol–imine tautomeric form. The molecule is approximately planar and intramolecular O—H···N hydrogen bonding generates an S(6) ring motif. C—H···π and offset π–π [3.726 (3) Å] interactions stabilize the structure. The F atoms are disordered approximately equally over two sites.

Related literature

For related literature, see: Moustakali-Mavridis *et al.* (1978); Umezawa *et al.* (1999); Hadjoudis *et al.* (1987); Sorell (1989); Gelling & Feringa (1990); Dutta *et al.* (1997); Bernstein *et al.* (1995); Ersanlı *et al.* (2004); Jacobsen (1993); Karadayı *et al.* (2003); Ligtenbarg *et al.* (1999); Pyrz *et al.* (1991); Xu *et al.* (1994); Şahin *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{12}NOF_3$
M_r = 279.26
Orthorhombic, $P2_12_12_1$
a = 6.1462 (4) Å
b = 14.2873 (8) Å
c = 14.8352 (13) Å

V = 1302.72 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 K
0.64 × 0.38 × 0.10 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED*; Stoe & Cie, 2002)
$T_{\min}$ = 0.940, $T_{\max}$ = 0.989

12218 measured reflections
1809 independent reflections
1382 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.257
S = 1.13
1809 reflections
183 parameters

60 restraints
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.64 e Å^{-3}
$\Delta\rho_{\min}$ = −0.56 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.90	2.618 (5)	146
C4—H4···$Cg2^{\text{i}}$	0.93	2.91	3.667 (5)	140
C11—H11···$Cg1^{\text{ii}}$	0.93	2.76	3.571 (5)	146

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2084).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Dutta, S. K., Ensling, J., Werner, R., Flörke, U., Haasse, W., Gütlich, P. & Nag, K. (1997). *Angew. Chem. Int. Ed. Engl.* **36**, 152–155.
Ersanlı, C. C., Odabaşoğlu, M., Albayrak, Ç. & Erdönmez, A. (2004). *Acta Cryst.* E**60**, o264–o266.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gelling, O. J. & Feringa, B. L. (1990). *J. Am. Chem. Soc.* **112**, 7599–7604.
Hadjoudis, E., Vittorakis, M. & Moustakali-Mavridis, I. (1987). *Tetrahedron*, **43**, 1345–1360.
Jacobsen, E. N. (1993). *Catalytic Asymmetric Synthesis*, edited by I. Ojima. New York: VCH.
Karadayı, N., Gözüyeşil, S., Güzel, B. & Büyükgüngör, O. (2003). *Acta Cryst.* E**59**, o161–o163.
Ligtenbarg, A. G. J., Hage, R., Meetsma, A. & Feringa, B. L. (1999). *J. Chem. Soc. Perkin Trans. 2*, pp. 807–812.
Moustakali-Mavridis, I., Hadjoudis, E. & Mavridis, A. (1978). *Acta Cryst.* B**34**, 3709–3715.
Pyrz, J. W., Pan, X., Britton, D. & Que, L. (1991). *Inorg. Chem.* **30**, 3461–3464.
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.
Sorell, T. N. (1989). *Tetrahedron*, **45**, 3–68.
Stoe & Cie (2002). *X-RED* and *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Umezawa, Y., Tsuboyama, S., Takahashi, H., Uzawa, J. & Nishio, M. (1999). *Tetrahedron*, **55**, 10047–10056.
Xu, X.-X., You, X.-Z., Sun, Z.-F., Wang, X. & Liu, H.-X. (1994). *Acta Cryst.* C**50**, 1169–1171.

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supplementary materials

Acta Cryst. (2007). E**63**, o3555 [**doi:10.1107/S1600536807030310**]

(*E*)-2-Methyl-6-[3-(trifluoromethyl)phenyliminomethyl]phenol

A. Akkaya, F. Ersahin, E. Agar, I. Senel and O. Büyükgüngör

Comment

Schiff base compounds are often used as ligands in coordination chemistry because they are generally known for their metal binding ability, and, in particular, salicylaldimines are useful for the synthesis of transition metal complexes. Some examples include Cu, Fe and Mn complexes (Sorell, 1989; Gelling & Feringa, 1990; Dutta *et al.*, 1997; Pyrz *et al.*, 1991; Jacobsen, 1993). Also, N-substituted salicylaldimines are of interest because of their thermochromism and photochromism in the solid state, which may involve reversible proton transfer from the hydroxyl O atom to the imine N atom (Moustakali-Mavridis *et al.*, 1978; Hadjoudis *et al.*, 1987; Xu *et al.*, 1994); charge transport occurs through intermolecular overlap of Π orbitals. Of the two tautomers, one is a phenol-imine structure and the other a keto-amine structure. Most crystal structures are of the phenol-imine tautomers (Ligtenbarg *et al.*, 1999).

The molecular structure of title compound is shown in Fig. 1. The C1–C7, C7═N1 and C8–N1 bond lengths are 1.432 (6) Å, 1.280 (5) Å and 1.417 (5) Å, respectively, and agree with the corresponding distances in *N*-[3,5-bis(trifluoromethyl)phenyl]salicylaldimine [1.439 (4) Å, 1.276 (4) Å and 1.417 (4) Å; Karadayı *et al.*, 2003]. The C2–O1 distance of 1.336 (5) Å is close to the corresponding distance in (*E*)-2-methoxy-6-[(2-trifluoromethylphenylimino) methyl]phenol [1.346 (4) Å, Şahin *et al.*, 2005]. There is a strong intramolecular O–H···N hydrogen bond in (I) (Table 1), which is a common feature of phenol-imine systems. Fig. 1 also shows a strong intramolecular hydrogen bond (O1–H1···N1), which gives rise to a six-membered pseudo-ring (Bernstein *et al.*, 1995). The O1–N1 distance of 2.618 (5) Å is comparable to those observed for analogous hydrogen bonds in 2-[2-(Hydroxymethyl)phenyliminomethyl]-phenol [2.613 (4) Å; Ersanlı *et al.*, 2004]. The dihedral angle between the rings formed by atoms C1—C6 and C8—C13 is 2.2 (2)°. C–H···π intermolecular and π–π stacking interactions play an appreciable role in determining the conformations of organic compounds (Umezawa *et al.*, 1999). C–H···π interactions are reported in Table 1. Also, there are two weak π—π stacking interactions, $Cg(1)–Cg(2)^{i}$ and $Cg(2)–Cg(1)^{ii}$, with the same (symmetry related) centroid-to-centroid distance of 3.726 (3) Å [*Cg*(1) and *Cg*(2) are the centroids of rings C1–C6 and C8–C13, respectively; symmetry codes: (i): −1+*X*,Y,*Z* and (ii): 1+*X*,Y,*Z*]. These interactions result in the structure packing in layers in the [100] direction.

Experimental

The compound (*E*)-2-methyl-6-[(3-(trifluoromethyl)phenylimino)methyl] phenol was prepared by refluxing a mixture of a solution containing 3-methylsalicylaldehyde (0.1 ml, 0.82 mmol) in 20 ml e thanol and a solution containing 3-aminobenzotrifluoride (0.13 g, 0.82 mmol) in 20 ml e thanol. The reaction mixture was stirred for 2 h under reflux. Crystals of (*E*)-2-methyl-6-[(3-(trifluoromethyl)phenylimino)methyl] phenol suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield 62%; m.p. 361–363 K).

Refinement

The high s.u. values and high displacement parameters of some atoms in the molecule are likely caused by disorder. The CF_3 group shows rotational disorder. The disordered trifluoromethyl F atoms were refined anisotropically, with geometrical and displacement parameter restraints for the two sets of positions; the refined occupancy factors are 0.494 (5) and 0.506 (5).

Refinement of H atoms was carried out using a riding model, with distances constrained to 0.82 Å for the OH group, 0.93 Å for aromatic CH, 0.98 Å for methyl CH and 0.96 Å for methyl CH_3. U_{iso}(H) parameters were set to 1.2U_{eq}(carrier atom) for aromatic CH and methine CH, and 1.5U_{eq}(carrier atom) for OH and methyl CH_3.

Figures

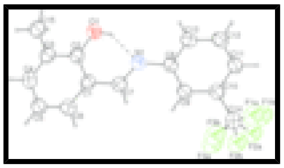

Fig. 1. A view of (I), with the atom-numbering scheme and displacement ellipsoids at the 40% probability level.

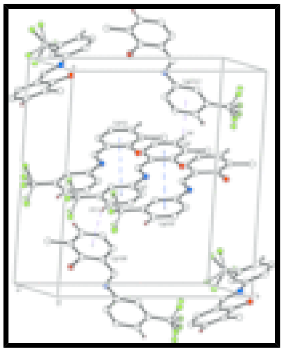

Fig. 2. C–H···π interactions and π–π stacking (dashed lines). H atoms not participating in hydrogen bonding have been omitted for clarity. [symmetry codes; (i):1+*X*,Y,*Z*; (ii):-1+*X*,Y,*Z*; (iii):-3/2-*X*,1-Y,1/2+*Z*; (iv):1/2-*X*,1-Y,-1/2+*Z*]

(*E*)-2-Methyl-6-[3-(trifluoromethyl)phenyliminomethyl]phenol

Crystal data

$C_{15}H_{12}NOF_3$	D_x = 1.424 Mg m^{-3}
M_r = 279.26	Melting point: 361-363 K
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 12218 reflections
a = 6.1462 (4) Å	θ = 2.0–28.0°
b = 14.2873 (8) Å	μ = 0.12 mm^{-1}
c = 14.8352 (13) Å	*T* = 296 K
V = 1302.72 (16) Å^3	Plate, light brown
Z = 4	0.64 × 0.38 × 0.10 mm
F_{000} = 576	

Data collection

Stoe IPDSII diffractometer	1809 independent reflections
Radiation source: sealed X-ray tube,12x0.4 mm long-fine focus	1382 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{\text{int}} = 0.054$
$T = 296$ K	$\theta_{\text{max}} = 27.9°$
rotation method scans	$\theta_{\text{min}} = 2.0°$
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	$h = -8\rightarrow8$
$T_{\text{min}} = 0.940$, $T_{\text{max}} = 0.989$	$k = -18\rightarrow18$
12218 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.076$	H-atom parameters constrained
$wR(F^2) = 0.257$	$w = 1/[\sigma^2(F_o^2) + (0.1762P)^2 + 0.1334P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1809 reflections	$\Delta\rho_{\text{max}} = 0.64$ e Å^{-3}
183 parameters	$\Delta\rho_{\text{min}} = -0.56$ e Å^{-3}
60 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.047 (18)

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
C1	0.2623 (7)	0.4947 (3)	0.5940 (3)	0.0517 (9)	
C2	0.1767 (7)	0.5864 (3)	0.6013 (3)	0.0526 (9)	

C3	−0.0192 (8)	0.6022 (3)	0.6485 (3)	0.0600 (11)	
C4	−0.1198 (8)	0.5266 (3)	0.6884 (3)	0.0624 (11)	
H4	−0.2468	0.5367	0.7210	0.075*	
C5	−0.0406 (8)	0.4364 (3)	0.6819 (3)	0.0619 (11)	
H5	−0.1142	0.3867	0.7086	0.074*	
C6	0.1491 (8)	0.4216 (3)	0.6353 (3)	0.0594 (10)	
H6	0.2039	0.3610	0.6311	0.071*	
C7	0.4560 (7)	0.4760 (3)	0.5434 (3)	0.0537 (9)	
H7	0.5103	0.4152	0.5427	0.064*	
C8	0.7465 (6)	0.5190 (3)	0.4482 (3)	0.0487 (8)	
C9	0.8360 (7)	0.4299 (3)	0.4367 (3)	0.0530 (9)	
H9	0.7688	0.3783	0.4628	0.064*	
C10	1.0232 (7)	0.4181 (3)	0.3868 (3)	0.0517 (9)	
C11	1.1236 (7)	0.4940 (3)	0.3455 (3)	0.0573 (10)	
H11	1.2494	0.4858	0.3116	0.069*	
C12	1.0328 (8)	0.5821 (3)	0.3558 (3)	0.0627 (11)	
H12	1.0975	0.6335	0.3282	0.075*	
C13	0.8490 (8)	0.5941 (3)	0.4062 (3)	0.0575 (10)	
H13	0.7910	0.6538	0.4126	0.069*	
C14	1.1204 (8)	0.3245 (3)	0.3759 (3)	0.0647 (11)	
C15	−0.1111 (10)	0.6981 (3)	0.6536 (4)	0.0804 (16)	
H15A	−0.1700	0.7152	0.5959	0.121*	
H15B	0.0016	0.7414	0.6699	0.121*	
H15C	−0.2244	0.6998	0.6981	0.121*	
F1A	1.3306 (15)	0.3212 (7)	0.3954 (7)	0.0894 (11)	0.494 (8)
F2A	1.1093 (16)	0.2935 (5)	0.2898 (6)	0.0894 (11)	0.494 (8)
F3A	1.0319 (15)	0.2600 (5)	0.4290 (6)	0.0894 (11)	0.494 (8)
F1B	1.3337 (15)	0.3227 (7)	0.3589 (7)	0.0894 (11)	0.506 (8)
F2B	1.0222 (15)	0.2705 (5)	0.3169 (6)	0.0894 (11)	0.506 (8)
F3B	1.1159 (15)	0.2748 (5)	0.4569 (5)	0.0894 (11)	0.506 (8)
N1	0.5574 (6)	0.5394 (2)	0.4993 (2)	0.0535 (8)	
O1	0.2753 (5)	0.6596 (2)	0.5630 (3)	0.0673 (10)	
H1	0.3906	0.6426	0.5405	0.101*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0514 (18)	0.0513 (18)	0.052 (2)	−0.0010 (16)	−0.0029 (18)	−0.0039 (15)
C2	0.0508 (19)	0.0510 (19)	0.056 (2)	0.0015 (16)	0.0000 (18)	0.0016 (16)
C3	0.059 (2)	0.063 (2)	0.059 (2)	0.0042 (19)	−0.002 (2)	−0.0033 (18)
C4	0.054 (2)	0.079 (3)	0.054 (2)	−0.001 (2)	0.005 (2)	0.002 (2)
C5	0.064 (2)	0.064 (2)	0.057 (2)	−0.011 (2)	0.005 (2)	0.0021 (19)
C6	0.063 (2)	0.054 (2)	0.061 (2)	−0.0007 (19)	0.002 (2)	0.0024 (18)
C7	0.0536 (19)	0.0514 (18)	0.056 (2)	0.0008 (17)	0.0018 (18)	−0.0022 (16)
C8	0.0451 (16)	0.0493 (18)	0.0518 (19)	−0.0039 (16)	−0.0025 (17)	0.0029 (15)
C9	0.0489 (19)	0.0518 (19)	0.058 (2)	−0.0040 (17)	0.0042 (18)	0.0064 (17)
C10	0.0499 (19)	0.0541 (19)	0.0512 (19)	−0.0034 (17)	0.0004 (17)	0.0008 (16)
C11	0.053 (2)	0.062 (2)	0.057 (2)	−0.0048 (19)	0.0074 (18)	0.0025 (18)

C12	0.069 (3)	0.055 (2)	0.064 (2)	−0.011 (2)	0.006 (2)	0.0072 (19)
C13	0.061 (2)	0.0479 (18)	0.063 (2)	−0.0026 (18)	−0.002 (2)	0.0035 (17)
C14	0.062 (2)	0.064 (2)	0.068 (3)	−0.001 (2)	0.011 (2)	−0.003 (2)
C15	0.076 (3)	0.062 (3)	0.103 (4)	0.014 (2)	0.023 (3)	0.000 (3)
F1A	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
F2A	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
F3A	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
F1B	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
F2B	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
F3B	0.094 (2)	0.0753 (15)	0.099 (3)	0.0152 (14)	0.003 (2)	−0.0061 (17)
N1	0.0489 (16)	0.0511 (16)	0.0605 (19)	0.0011 (14)	−0.0017 (15)	0.0037 (14)
O1	0.0653 (19)	0.0497 (15)	0.087 (2)	0.0024 (14)	0.0152 (18)	0.0053 (14)

Geometric parameters (Å, °)

C1—C6	1.397 (6)	C9—H9	0.9300
C1—C2	1.416 (5)	C10—C11	1.390 (6)
C1—C7	1.432 (6)	C10—C14	1.473 (6)
C2—O1	1.335 (5)	C11—C12	1.386 (6)
C2—C3	1.411 (6)	C11—H11	0.9300
C3—C4	1.378 (6)	C12—C13	1.365 (7)
C3—C15	1.484 (6)	C12—H12	0.9300
C4—C5	1.381 (7)	C13—H13	0.9300
C4—H4	0.9300	C14—F2B	1.312 (9)
C5—C6	1.372 (6)	C14—F1A	1.325 (10)
C5—H5	0.9300	C14—F3A	1.329 (9)
C6—H6	0.9300	C14—F1B	1.336 (10)
C7—N1	1.280 (5)	C14—F2A	1.354 (9)
C7—H7	0.9300	C14—F3B	1.396 (9)
C8—C13	1.392 (5)	C15—H15A	0.9600
C8—C9	1.397 (6)	C15—H15B	0.9600
C8—N1	1.417 (5)	C15—H15C	0.9600
C9—C10	1.378 (6)	O1—H1	0.8200
C6—C1—C2	118.3 (4)	C13—C12—C11	120.5 (4)
C6—C1—C7	120.3 (4)	C13—C12—H12	119.7
C2—C1—C7	121.4 (4)	C11—C12—H12	119.7
O1—C2—C3	118.3 (4)	C12—C13—C8	121.5 (4)
O1—C2—C1	121.6 (4)	C12—C13—H13	119.2
C3—C2—C1	120.2 (4)	C8—C13—H13	119.2
C4—C3—C2	118.1 (4)	F2B—C14—F1A	125.0 (7)
C4—C3—C15	122.1 (4)	F2B—C14—F3A	78.4 (6)
C2—C3—C15	119.8 (4)	F1A—C14—F3A	104.2 (7)
C3—C4—C5	122.9 (4)	F2B—C14—F1B	108.3 (7)
C3—C4—H4	118.5	F3A—C14—F1B	120.0 (7)
C5—C4—H4	118.5	F1A—C14—F2A	104.1 (6)
C6—C5—C4	118.6 (4)	F3A—C14—F2A	108.2 (6)
C6—C5—H5	120.7	F1B—C14—F2A	82.2 (6)
C4—C5—H5	120.7	F2B—C14—F3B	105.4 (6)
C5—C6—C1	121.9 (4)	F1A—C14—F3B	79.2 (6)

C5—C6—H6	119.0	F1B—C14—F3B	99.9 (7)
C1—C6—H6	119.0	F2A—C14—F3B	130.2 (6)
N1—C7—C1	122.7 (4)	F2B—C14—C10	114.8 (5)
N1—C7—H7	118.6	F1A—C14—C10	113.8 (6)
C1—C7—H7	118.6	F3A—C14—C10	113.5 (5)
C13—C8—C9	118.0 (4)	F1B—C14—C10	115.9 (6)
C13—C8—N1	116.9 (3)	F2A—C14—C10	112.4 (5)
C9—C8—N1	125.1 (3)	F3B—C14—C10	111.0 (5)
C10—C9—C8	120.4 (4)	C3—C15—H15A	109.5
C10—C9—H9	119.8	C3—C15—H15B	109.5
C8—C9—H9	119.8	H15A—C15—H15B	109.5
C9—C10—C11	120.8 (4)	C3—C15—H15C	109.5
C9—C10—C14	120.6 (4)	H15A—C15—H15C	109.5
C11—C10—C14	118.6 (4)	H15B—C15—H15C	109.5
C12—C11—C10	118.8 (4)	C7—N1—C8	121.9 (3)
C12—C11—H11	120.6	C2—O1—H1	109.5
C10—C11—H11	120.6		

C6—C1—C2—O1	−179.5 (4)	C14—C10—C11—C12	−179.9 (4)
C7—C1—C2—O1	−1.5 (6)	C10—C11—C12—C13	0.5 (7)
C6—C1—C2—C3	−0.6 (6)	C11—C12—C13—C8	−0.3 (7)
C7—C1—C2—C3	177.5 (4)	C9—C8—C13—C12	−0.7 (6)
O1—C2—C3—C4	−179.6 (4)	N1—C8—C13—C12	179.7 (4)
C1—C2—C3—C4	1.4 (6)	C9—C10—C14—F2B	77.6 (7)
O1—C2—C3—C15	0.8 (6)	C11—C10—C14—F2B	−102.1 (7)
C1—C2—C3—C15	−178.2 (5)	C9—C10—C14—F1A	−129.0 (6)
C2—C3—C4—C5	−1.7 (7)	C11—C10—C14—F1A	51.3 (8)
C15—C3—C4—C5	177.8 (5)	C9—C10—C14—F3A	−10.1 (8)
C3—C4—C5—C6	1.3 (7)	C11—C10—C14—F3A	170.2 (6)
C4—C5—C6—C1	−0.4 (7)	C9—C10—C14—F1B	−154.9 (6)
C2—C1—C6—C5	0.1 (6)	C11—C10—C14—F1B	25.4 (8)
C7—C1—C6—C5	−178.0 (4)	C9—C10—C14—F2A	113.0 (6)
C6—C1—C7—N1	175.1 (4)	C11—C10—C14—F2A	−66.7 (7)
C2—C1—C7—N1	−2.9 (6)	C9—C10—C14—F3B	−41.9 (7)
C13—C8—C9—C10	1.6 (6)	C11—C10—C14—F3B	138.4 (6)
N1—C8—C9—C10	−178.8 (4)	C1—C7—N1—C8	−178.7 (3)
C8—C9—C10—C11	−1.5 (6)	C13—C8—N1—C7	−177.2 (4)
C8—C9—C10—C14	178.8 (4)	C9—C8—N1—C7	3.2 (6)
C9—C10—C11—C12	0.4 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.90	2.618 (5)	146
C4—H4···Cg2^{i}	0.93	2.91	3.667 (5)	140
C11—H11···Cg1^{ii}	0.93	2.76	3.571 (5)	146

Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*+1/2; (ii) −*x*+3/2, −*y*+1, *z*−1/2.

Fig. 1

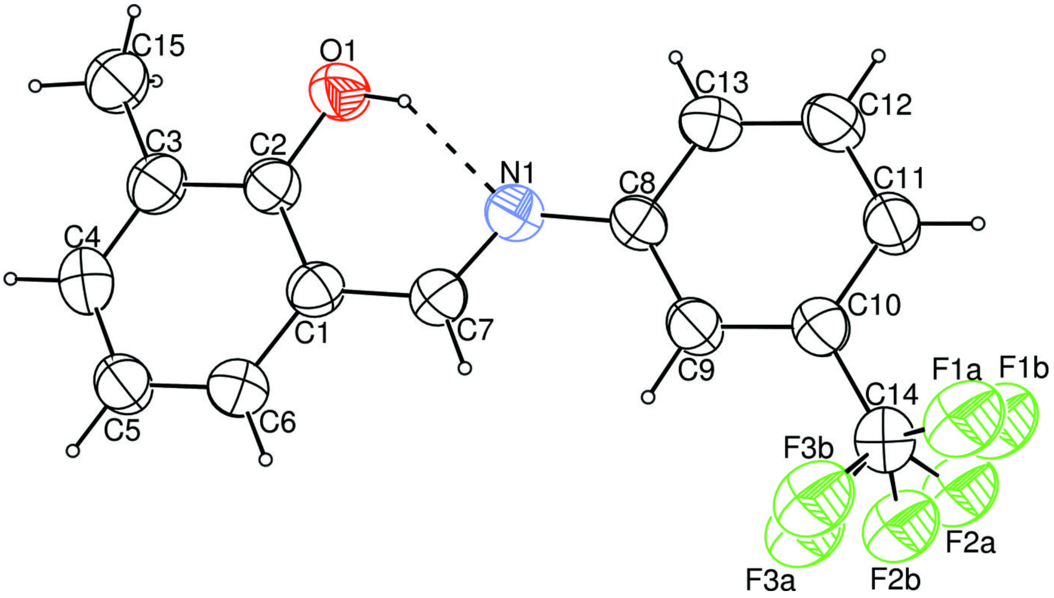
C15
O1
C13
C12
C3
C2
N1
C8
C11
C4
C10
C1
C7
C9
F1a
F1b
C14
C5
C6
F3b
F2a
F3a
F2b

Fig. 2