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Shaukat Shuja,[a] Saqib Ali,[a] Auke Meetsma,[b] Grant A. Broker[c] and Edward R. T. Tiekink[c]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, [b]Crystal Structure Center, Chemical Physics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands, and [c]Department of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA

Correspondence e-mail:
edward.tiekink@utsa.edu

Key indicators

Single-crystal X-ray study
$T = 100$ K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.046
wR factor = 0.139
Data-to-parameter ratio = 10.5

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

The crystal packing of the essentially planar molecules of the title compound, $C_{14}H_{10}F_3NO_2$, is stabilized by O—H⋯O hydrogen bonds and possible C—H⋯O and C—H⋯F interactions.

Comment

As part of our onging studies (Shuja *et al.*, 2006) of the structural aspects of hydroxy Schiff bases aimed towards the development of materials with superior optical properties and biological activities, we now report the synthesis and structure of the title compound, (I) (Fig. 1).

(I)
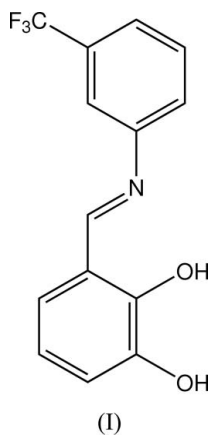
Molecules of compound (I) are essentially planar in the crystal structure, as manifested in the C6—N1—C8—C9
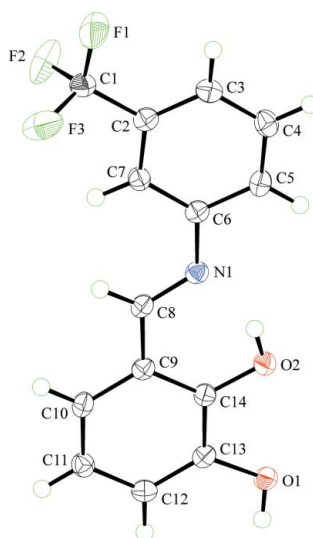
Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). Only the major component of the disordered CF_3 group is shown.

Figure 2
Chain formation *via* O—H···O (orange dashed lines) interactions along the *b* axis in the structure of (I). Color code: F atoms are shown in cyan, O atoms in red, N atoms in blue, C atoms in grey and H atoms in green. Only one disorder component is shown.

Figure 3
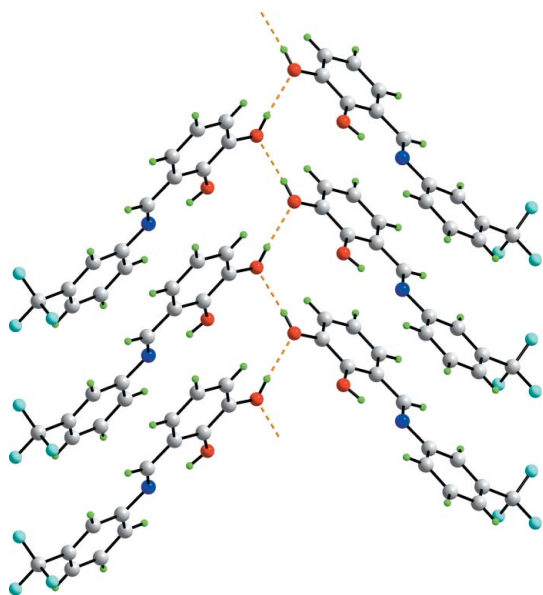Unit-cell contents of (I), viewed down the *c*-axis direction. Color code as for Fig. 2. The O—H···O (orange) and C—H···F (blue) interactions are shown as dashed lines. Only one disorder component is shown.

torsion angle of −179.13 (14) Å. Both intra- and inter-molecular O—H···O hydrogen bonds are noted in the structure (Table 1), with the latter leading to the formation of chains along the *b* axis (Fig. 2). Contacts between the chains are afforded by C—H···F interactions resulting in layers stacked along the *c* axis. The most prominent connection between layers is a C—H···O interaction.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O1^i	0.84	1.93	2.7510 (15)	165
O2—H2O···N1	0.84	1.81	2.596 (2)	154
C10—H10···F3^{ii}	0.95	2.53	3.380 (3)	149
C4—H4···O1^{iii}	0.95	2.61	3.392 (2)	140

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

All H atoms were placed geometrically (C—H = 0.95 Å and O—H = 0.84 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). The CF₃ group is disordered over two orientations in a 0.908 (4):0.092 (4) ratio.

Data collection: *SMART*, (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

Experimental

2,3-Dihydroxybenzaldehyde (0.5 g, 3.6 mmol) and 3-(trifluoromethyl)aniline (0.58 g, 3.6 mmol) in ethanol (40 ml) were heated under reflux for 2 h with stirring. The solution was cooled and kept in the dark. Orange–red crystals of (I) were collected after two days (m.p. 389–391 K).
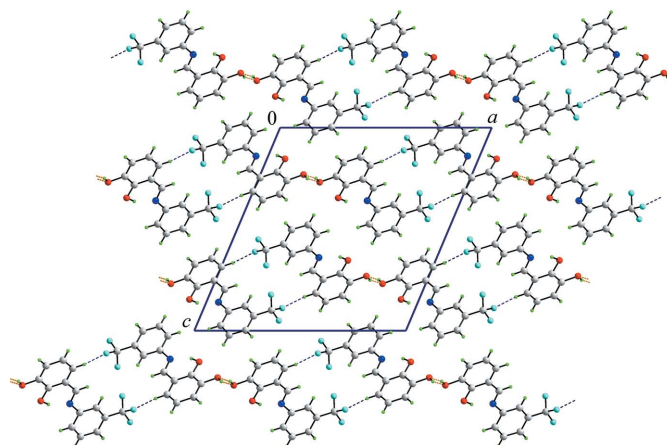
Crystal data

C₁₄H₁₀F₃NO₂	V = 1207.92 (12) Å³
M_r = 281.23	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 16.2463 (9) Å	μ = 0.14 mm⁻¹
b = 4.7716 (3) Å	T = 100 (2) K
c = 16.9199 (9) Å	0.49 × 0.41 × 0.22 mm
β = 112.939 (1)°	

Data collection

Bruker SMART CCD diffractometer	8910 measured reflections
	2109 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)	1870 reflections with $I > 2\sigma(I)$
T_{min} = 0.909, T_{max} = 0.971	R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046	201 parameters
$wR(F^2)$ = 0.139	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.49 e Å⁻³
2109 reflections	$\Delta\rho_{min}$ = −0.40 e Å⁻³

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supporting information

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3-[3-(Trifluoromethyl)phenyliminomethyl]benzene-1,2-diol

Crystal data

$C_{14}H_{10}F_3NO_2$	$F(000) = 576$
$M_r = 281.23$	$D_x = 1.546$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5078 reflections
$a = 16.2463$ (9) Å	$\theta = 2.6–29.5°$
$b = 4.7716$ (3) Å	$\mu = 0.14$ mm^{-1}
$c = 16.9199$ (9) Å	$T = 100$ K
$\beta = 112.939$ (1)°	Block, orange-red
$V = 1207.92$ (12) Å^3	$0.49 \times 0.41 \times 0.22$ mm
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	$T_{min} = 0.909$, $T_{max} = 0.971$
Radiation source: fine-focus sealed tube	8910 measured reflections
Graphite monochromator	2109 independent reflections
Detector resolution: 4096x4096 / 62x62 (binned 512) pixels mm^{-1}	1870 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.015$
Absorption correction: multi-scan (SADABS; Bruker, 2006)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
	$h = -19 \rightarrow 17$
	$k = 0 \rightarrow 5$
	$l = 0 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 0.695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	
2109 reflections	$(\Delta/\sigma)_{max} < 0.001$
201 parameters	$\Delta\rho_{max} = 0.49$ e Å^{-3}
8 restraints	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	

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 $F^2 > \sigma(F^2)$ 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	0.82417 (12)	0.3364 (4)	0.39916 (12)	0.0276 (4)	0.908 (4)
F1	0.87946 (12)	0.1499 (4)	0.45002 (11)	0.0580 (6)	0.908 (4)
F2	0.79056 (10)	0.2039 (5)	0.32209 (9)	0.0561 (6)	0.908 (4)
F3	0.87048 (13)	0.5458 (3)	0.38851 (18)	0.0816 (9)	0.908 (4)
C1A	0.82417 (12)	0.3364 (4)	0.39916 (12)	0.0276 (4)	0.092 (4)
F1A	0.8331 (15)	0.077 (2)	0.4117 (10)	0.108 (10)*	0.092 (4)
F2A	0.8099 (7)	0.389 (3)	0.3224 (6)	0.022 (4)*	0.092 (4)
F3A	0.8945 (9)	0.459 (4)	0.4482 (9)	0.062 (6)*	0.092 (4)
O1	0.29573 (8)	1.5909 (2)	0.26882 (8)	0.0247 (3)	
H1O	0.2706	1.7440	0.2496	0.037*	
O2	0.41465 (8)	1.1978 (3)	0.34631 (8)	0.0251 (3)	
H2O	0.4577	1.0850	0.3629	0.038*	
N1	0.55754 (9)	0.9236 (3)	0.35995 (9)	0.0214 (3)	
C2	0.75077 (11)	0.4256 (4)	0.42676 (11)	0.0227 (4)	
C3	0.74251 (11)	0.3013 (4)	0.49780 (11)	0.0243 (4)	
H3	0.7834	0.1607	0.5297	0.029*	
C4	0.67344 (12)	0.3867 (4)	0.52115 (11)	0.0265 (4)	
H4	0.6667	0.3036	0.5693	0.032*	
C5	0.61422 (12)	0.5926 (4)	0.47458 (11)	0.0240 (4)	
H5	0.5675	0.6501	0.4915	0.029*	
C6	0.62212 (11)	0.7168 (3)	0.40319 (11)	0.0204 (4)	
C7	0.69145 (11)	0.6307 (4)	0.37922 (11)	0.0219 (4)	
H7	0.6979	0.7120	0.3307	0.026*	
C8	0.56055 (11)	1.0658 (3)	0.29622 (11)	0.0209 (4)	
H8	0.6070	1.0300	0.2767	0.025*	
C9	0.49444 (11)	1.2791 (3)	0.25370 (11)	0.0200 (4)	
C10	0.50036 (11)	1.4337 (4)	0.18519 (11)	0.0226 (4)	
H10	0.5472	1.3949	0.1664	0.027*	
C11	0.43910 (12)	1.6407 (4)	0.14509 (11)	0.0231 (4)	
H11	0.4439	1.7443	0.0991	0.028*	
C12	0.36956 (11)	1.6977 (4)	0.17246 (11)	0.0219 (4)	
H12	0.3271	1.8397	0.1448	0.026*	
C13	0.36279 (11)	1.5480 (3)	0.23952 (11)	0.0205 (4)	
C14	0.42466 (11)	1.3369 (3)	0.28125 (11)	0.0200 (4)	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0277 (9)	0.0243 (9)	0.0321 (10)	0.0041 (7)	0.0132 (8)	0.0036 (8)
F1	0.0523 (10)	0.0809 (12)	0.0511 (10)	0.0462 (9)	0.0313 (9)	0.0318 (9)

F2	0.0430 (8)	0.0863 (16)	0.0454 (9)	0.0055 (9)	0.0242 (7)	−0.0207 (8)
F3	0.0755 (13)	0.0296 (8)	0.189 (3)	−0.0035 (8)	0.1056 (16)	0.0007 (11)
C1A	0.0277 (9)	0.0243 (9)	0.0321 (10)	0.0041 (7)	0.0132 (8)	0.0036 (8)
O1	0.0219 (6)	0.0231 (6)	0.0330 (7)	0.0024 (5)	0.0150 (5)	0.0023 (5)
O2	0.0249 (6)	0.0255 (7)	0.0290 (7)	0.0042 (5)	0.0150 (5)	0.0050 (5)
N1	0.0214 (7)	0.0201 (7)	0.0229 (7)	−0.0010 (6)	0.0089 (6)	−0.0022 (6)
C2	0.0212 (8)	0.0214 (8)	0.0240 (9)	−0.0026 (7)	0.0072 (7)	−0.0037 (7)
C3	0.0234 (9)	0.0229 (9)	0.0224 (9)	−0.0001 (7)	0.0043 (7)	0.0005 (7)
C4	0.0290 (9)	0.0295 (9)	0.0202 (9)	−0.0022 (7)	0.0086 (7)	0.0010 (7)
C5	0.0232 (9)	0.0284 (9)	0.0222 (9)	−0.0022 (7)	0.0106 (7)	−0.0036 (7)
C6	0.0194 (8)	0.0192 (8)	0.0209 (8)	−0.0027 (7)	0.0060 (7)	−0.0040 (7)
C7	0.0235 (9)	0.0219 (8)	0.0212 (9)	−0.0021 (7)	0.0097 (7)	−0.0007 (7)
C8	0.0190 (8)	0.0207 (8)	0.0241 (9)	−0.0024 (7)	0.0097 (7)	−0.0046 (7)
C9	0.0191 (8)	0.0193 (8)	0.0208 (8)	−0.0025 (7)	0.0070 (7)	−0.0040 (6)
C10	0.0220 (8)	0.0249 (9)	0.0240 (9)	−0.0034 (7)	0.0123 (7)	−0.0046 (7)
C11	0.0254 (9)	0.0233 (9)	0.0206 (9)	−0.0022 (7)	0.0089 (7)	−0.0007 (7)
C12	0.0205 (8)	0.0192 (8)	0.0227 (9)	−0.0017 (7)	0.0049 (7)	−0.0023 (7)
C13	0.0173 (8)	0.0201 (8)	0.0241 (9)	−0.0031 (7)	0.0081 (7)	−0.0049 (7)
C14	0.0198 (8)	0.0191 (8)	0.0215 (8)	−0.0046 (7)	0.0087 (7)	−0.0033 (7)

Geometric parameters (Å, º)

C1—F3	1.305 (2)	C3—H3	0.9500
C1—F1	1.318 (2)	C4—C5	1.386 (3)
C1—F2	1.358 (2)	C4—H4	0.9500
C1—C2	1.502 (2)	C5—C6	1.395 (2)
C1A—F1A	1.256 (11)	C5—H5	0.9500
C1A—F2A	1.251 (9)	C6—C7	1.399 (2)
C1A—F3A	1.264 (10)	C7—H7	0.9500
C1A—C2	1.502 (2)	C8—C9	1.451 (2)
F1A—F2A	2.048 (16)	C8—H8	0.9500
O1—C13	1.377 (2)	C9—C10	1.408 (2)
O1—H1O	0.84	C9—C14	1.411 (2)
O2—C14	1.349 (2)	C10—C11	1.378 (2)
O2—H2O	0.84	C10—H10	0.9500
N1—C8	1.291 (2)	C11—C12	1.405 (2)
N1—C6	1.418 (2)	C11—H11	0.9500
C2—C3	1.393 (3)	C12—C13	1.381 (2)
C2—C7	1.389 (2)	C12—H12	0.9500
C3—C4	1.388 (3)	C13—C14	1.403 (2)
F3—C1—F1	108.92 (18)	C6—C5—H5	119.5
F3—C1—F2	105.16 (18)	C5—C6—C7	118.82 (16)
F1—C1—F2	103.26 (17)	C5—C6—N1	116.29 (15)
F3—C1—C2	113.36 (16)	C7—C6—N1	124.88 (15)
F1—C1—C2	114.21 (16)	C2—C7—C6	119.62 (16)
F2—C1—C2	111.09 (15)	C2—C7—H7	120.2
F1A—C1A—F2A	109.5 (6)	C6—C7—H7	120.2

F1A—C1A—F3A	109.3 (6)	N1—C8—C9	121.42 (15)
F2A—C1A—F3A	110.1 (5)	N1—C8—H8	119.3
F1A—C1A—C2	106.3 (10)	C9—C8—H8	119.3
F2A—C1A—C2	114.7 (5)	C10—C9—C14	119.40 (16)
F3A—C1A—C2	106.8 (7)	C10—C9—C8	120.05 (15)
C13—O1—H1O	108.8	C14—C9—C8	120.54 (15)
C14—O2—H2O	103.9	C11—C10—C9	120.83 (16)
C8—N1—C6	122.38 (15)	C11—C10—H10	119.6
C3—C2—C7	121.41 (16)	C9—C10—H10	119.6
C3—C2—C1A	120.20 (16)	C10—C11—C12	119.73 (16)
C7—C2—C1A	118.38 (16)	C10—C11—H11	120.1
C3—C2—C1	120.20 (16)	C12—C11—H11	120.1
C7—C2—C1	118.38 (16)	C13—C12—C11	120.16 (16)
C4—C3—C2	118.76 (16)	C13—C12—H12	119.9
C4—C3—H3	120.6	C11—C12—H12	119.9
C2—C3—H3	120.6	O1—C13—C12	123.12 (15)
C5—C4—C3	120.35 (17)	O1—C13—C14	115.96 (15)
C5—C4—H4	119.8	C12—C13—C14	120.91 (15)
C3—C4—H4	119.8	O2—C14—C13	118.24 (15)
C4—C5—C6	121.04 (16)	O2—C14—C9	122.79 (15)
C4—C5—H5	119.5	C13—C14—C9	118.97 (15)
F3A—C1A—F1A—F2A	−120.7 (9)	C4—C5—C6—C7	−0.2 (3)
C2—C1A—F1A—F2A	124.4 (7)	C4—C5—C6—N1	179.55 (15)
F3A—C1A—F2A—F1A	120.2 (9)	C8—N1—C6—C5	175.80 (15)
C2—C1A—F2A—F1A	−119.3 (11)	C8—N1—C6—C7	−4.4 (3)
F1A—C1A—C2—C3	36.9 (9)	C3—C2—C7—C6	0.5 (3)
F2A—C1A—C2—C3	158.1 (7)	C1A—C2—C7—C6	179.66 (15)
F3A—C1A—C2—C3	−79.7 (8)	C1—C2—C7—C6	179.66 (15)
F1A—C1A—C2—C7	−142.3 (8)	C5—C6—C7—C2	−0.2 (2)
F2A—C1A—C2—C7	−21.1 (7)	N1—C6—C7—C2	−179.99 (15)
F3A—C1A—C2—C7	101.1 (8)	C6—N1—C8—C9	−179.13 (14)
F1A—C1A—C2—C1	0 (100)	N1—C8—C9—C10	179.02 (15)
F2A—C1A—C2—C1	0 (100)	N1—C8—C9—C14	0.0 (2)
F3A—C1A—C2—C1	0 (38)	C14—C9—C10—C11	0.2 (2)
F3—C1—C2—C3	−129.1 (2)	C8—C9—C10—C11	−178.80 (15)
F1—C1—C2—C3	−3.5 (3)	C9—C10—C11—C12	−0.3 (3)
F2—C1—C2—C3	112.7 (2)	C10—C11—C12—C13	0.3 (2)
F3—C1—C2—C7	51.7 (3)	C11—C12—C13—O1	−179.19 (15)
F1—C1—C2—C7	177.24 (17)	C11—C12—C13—C14	−0.1 (2)
F2—C1—C2—C7	−66.5 (2)	O1—C13—C14—O2	−0.9 (2)
F3—C1—C2—C1A	0 (42)	C12—C13—C14—O2	180.00 (14)
F1—C1—C2—C1A	0 (100)	O1—C13—C14—C9	179.13 (14)
F2—C1—C2—C1A	0 (100)	C12—C13—C14—C9	0.0 (2)
C7—C2—C3—C4	−0.2 (3)	C10—C9—C14—O2	179.97 (15)
C1A—C2—C3—C4	−179.42 (16)	C8—C9—C14—O2	−1.0 (2)
C1—C2—C3—C4	−179.42 (16)	C10—C9—C14—C13	0.0 (2)
C2—C3—C4—C5	−0.2 (3)	C8—C9—C14—C13	178.95 (14)

| C3—C4—C5—C6 | 0.5 (3) | | | |

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1O⋯O1[i]	0.84	1.93	2.7510 (15)	165
O2—H2O⋯N1	0.84	1.81	2.596 (2)	154
C10—H10⋯F3[ii]	0.95	2.53	3.380 (3)	149
C4—H4⋯O1[iii]	0.95	2.61	3.392 (2)	140

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