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4′-Fluoro-2′-hydroxyacetophenone

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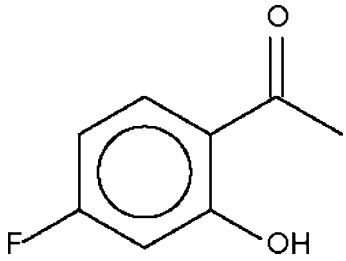
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.128; data-to-parameter ratio = 12.5.

The title compound, $C_8H_7FO_2$, crystallizes as discrete molecules, the conformation of which may be influenced by an intramolecular hydroxy–carbonyl O—H···O hydrogen bond.

Related literature

For the crystal structures of other substituted acetophenones, see: Filarowski *et al.* (2004, 2005); Hibbs *et al.* (2003); Huang *et al.* (2004); Ng (2007); Xu *et al.* (2005).



Experimental

Crystal data

$C_8H_7FO_2$
M_r = 154.14
Monoclinic, $P2_1/n$
a = 3.7978 (1) Å
b = 14.2421 (3) Å
c = 13.0092 (3) Å
β = 91.884 (2)°
V = 703.27 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100 (2) K
0.16 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
8762 measured reflections
1601 independent reflections
1224 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.05
1601 reflections
128 parameters
7 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.857 (10)	1.76 (1)	2.554 (2)	154 (2)

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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, 2008).

We thank the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2605).

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supporting information

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4′-Fluoro-2′-hydroxyacetophenone

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S1. Comment

Acetopheonone is a liquid at room temperature. If a small substituent such as 5′-bromo (Ng, 2007), 5′-chloro (Filarowski *et al.*, 2004), 6′-hydroxy (Huang *et al.*, 2004), 5′-nitro (Hibbs *et al.*, 2003), 4′-methoxy (Filarowski *et al.*, 2005; Xu *et al.*, 2005) or 6′-methoxy (Filarowski *et al.*, 2005) is present the compounds exists as crystalline solids. The compound (I) containing the reltively smaller F substituent sublimes at room temperature. The structure contains discrete molecules (Fig. 1), in which the conformation may be influenced by an intramolecular hydrogen bond between the hydroxy and carbonyl groups.

S2. Experimental

The compound was purchased from Aldrich Chemical Company; the chemical exists as prismatic crystals.

S3. Refinement

All H-atoms were located in a difference Fourier map, and were refined with distance restraints of C—H 0.99±0.01 Å and O–H 0.84±0.01 Å. Their temperature factors were freely refined.

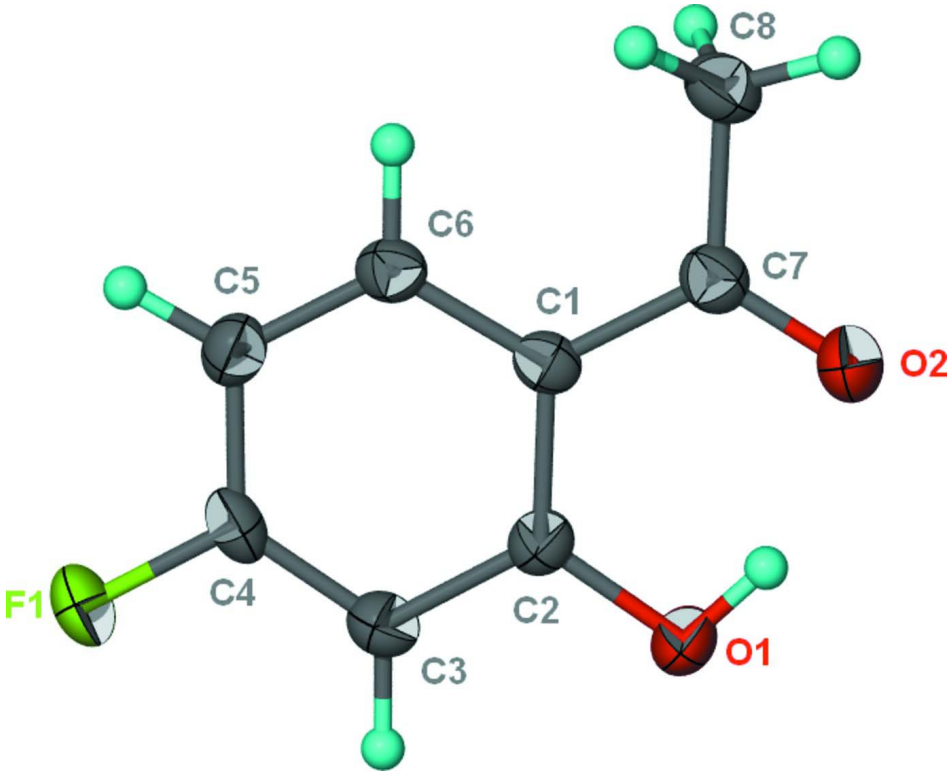

Figure 1

70% Probability thermal ellipsoid plot of 4′-fluoro-2′-hydroxyacetophenone. Hydrogen atoms are drawn as spheres of arbitrary radius.

4-fluoro-2-hydroxybenzaldehyde

Crystal data

$C_8H_7FO_2$
$M_r = 154.14$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 3.7978$ (1) Å
$b = 14.2421$ (3) Å
$c = 13.0092$ (3) Å
$\beta = 91.884$ (2)°
$V = 703.27$ (3) Å^3
$Z = 4$
$F(000) = 320$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1854 reflections
$\theta = 2.9$–26.4°
$\mu = 0.12$ mm^{-1}
$T = 100$ K
Prism, colorless
0.16 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8762 measured reflections
1601 independent reflections
1224 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -4 \rightarrow 4$
$k = -18 \rightarrow 18$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.127$
$S = 1.05$
1601 reflections
128 parameters
7 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.0798P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.1828 (3)	0.50469 (6)	0.65495 (7)	0.0319 (3)
O1	0.4466 (3)	0.72547 (8)	0.40329 (8)	0.0325 (3)
O2	0.7055 (3)	0.88271 (8)	0.46250 (8)	0.0320 (3)
C1	0.5542 (4)	0.76649 (10)	0.58170 (11)	0.0196 (3)
C2	0.4380 (4)	0.70349 (10)	0.50349 (11)	0.0211 (3)
C3	0.3106 (4)	0.61483 (10)	0.52868 (11)	0.0229 (3)
C4	0.3051 (4)	0.59128 (10)	0.63045 (12)	0.0225 (4)
C5	0.4165 (4)	0.64954 (10)	0.71015 (11)	0.0235 (4)
C6	0.5398 (4)	0.73716 (10)	0.68410 (11)	0.0216 (4)
C7	0.6909 (4)	0.85914 (10)	0.55377 (11)	0.0227 (4)
C8	0.8132 (5)	0.92675 (11)	0.63595 (12)	0.0267 (4)
H1	0.519 (6)	0.7824 (9)	0.4037 (19)	0.066 (8)*
H3	0.221 (5)	0.5733 (10)	0.4729 (11)	0.029 (5)*
H5	0.412 (5)	0.6279 (11)	0.7807 (8)	0.023 (4)*
H6	0.616 (4)	0.7801 (10)	0.7398 (10)	0.024 (4)*
H81	0.602 (4)	0.9492 (14)	0.6716 (15)	0.051 (6)*
H82	0.968 (4)	0.8980 (12)	0.6899 (12)	0.033 (5)*
H83	0.937 (5)	0.9790 (11)	0.6047 (15)	0.044 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0427 (6)	0.0200 (5)	0.0331 (5)	−0.0081 (4)	0.0043 (4)	0.0043 (4)
O1	0.0514 (8)	0.0275 (6)	0.0182 (6)	−0.0115 (6)	−0.0021 (5)	0.0018 (4)
O2	0.0457 (8)	0.0252 (6)	0.0254 (6)	−0.0091 (5)	0.0038 (5)	0.0027 (4)
C1	0.0191 (8)	0.0176 (7)	0.0221 (7)	0.0013 (5)	0.0012 (6)	−0.0019 (5)
C2	0.0223 (8)	0.0221 (8)	0.0187 (7)	−0.0003 (6)	0.0002 (6)	0.0003 (5)
C3	0.0235 (8)	0.0207 (7)	0.0244 (8)	−0.0012 (6)	−0.0003 (6)	−0.0023 (6)
C4	0.0227 (8)	0.0146 (7)	0.0304 (8)	−0.0005 (6)	0.0045 (6)	0.0030 (6)
C5	0.0266 (9)	0.0240 (8)	0.0201 (7)	0.0020 (6)	0.0028 (6)	0.0026 (6)
C6	0.0226 (8)	0.0205 (7)	0.0217 (7)	0.0022 (6)	0.0007 (6)	−0.0022 (5)
C7	0.0231 (8)	0.0204 (7)	0.0247 (8)	0.0006 (6)	0.0021 (6)	−0.0004 (6)
C8	0.0277 (9)	0.0220 (8)	0.0304 (8)	−0.0035 (6)	0.0026 (7)	−0.0032 (6)

Geometric parameters (Å, º)

F1—C4	1.3594 (16)	C3—H3	0.988 (9)
O1—C2	1.3420 (17)	C4—C5	1.383 (2)
O1—H1	0.857 (10)	C5—C6	1.379 (2)
O2—C7	1.2370 (18)	C5—H5	0.969 (9)
C1—C6	1.399 (2)	C6—H6	0.984 (9)
C1—C2	1.416 (2)	C7—C8	1.501 (2)
C1—C7	1.468 (2)	C8—H81	0.993 (10)
C2—C3	1.395 (2)	C8—H82	0.989 (9)
C3—C4	1.367 (2)	C8—H83	0.977 (10)
C2—O1—H1	103.5 (17)	C6—C5—H5	122.5 (10)
C6—C1—C2	118.29 (13)	C4—C5—H5	120.3 (10)
C6—C1—C7	121.96 (13)	C5—C6—C1	121.90 (13)
C2—C1—C7	119.74 (13)	C5—C6—H6	118.4 (10)
O1—C2—C3	117.32 (13)	C1—C6—H6	119.7 (10)
O1—C2—C1	122.21 (13)	O2—C7—C1	120.59 (13)
C3—C2—C1	120.47 (13)	O2—C7—C8	119.14 (14)
C4—C3—C2	117.78 (14)	C1—C7—C8	120.27 (13)
C4—C3—H3	123.3 (11)	C7—C8—H81	107.6 (13)
C2—C3—H3	118.9 (10)	C7—C8—H82	113.7 (11)
F1—C4—C3	117.77 (13)	H81—C8—H82	105.8 (17)
F1—C4—C5	117.83 (13)	C7—C8—H83	109.5 (12)
C3—C4—C5	124.40 (14)	H81—C8—H83	111.0 (18)
C6—C5—C4	117.17 (13)	H82—C8—H83	109.2 (17)
C6—C1—C2—O1	−179.20 (14)	C3—C4—C5—C6	0.2 (2)
C7—C1—C2—O1	−0.3 (2)	C4—C5—C6—C1	−0.3 (2)
C6—C1—C2—C3	0.4 (2)	C2—C1—C6—C5	0.0 (2)
C7—C1—C2—C3	179.37 (14)	C7—C1—C6—C5	−178.94 (14)
O1—C2—C3—C4	179.15 (14)	C6—C1—C7—O2	178.92 (14)
C1—C2—C3—C4	−0.5 (2)	C2—C1—C7—O2	0.0 (2)
C2—C3—C4—F1	−179.64 (13)	C6—C1—C7—C8	−1.4 (2)
C2—C3—C4—C5	0.2 (2)	C2—C1—C7—C8	179.68 (14)
F1—C4—C5—C6	−179.97 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.86 (1)	1.76 (1)	2.554 (2)	154 (2)