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# 4′-Fluoro-2′-hydroxyacetophenone

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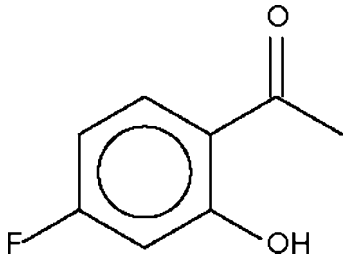
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.128; data-to-parameter ratio = 12.5.

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
$\beta$ = 91.884 (2)°
$V$ = 703.27 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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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# supplementary materials

*Acta Cryst.* (2008). E**64**, o916 [ **doi:10.1107/S1600536808011173** ]

# 4'-Fluoro-2'-hydroxyacetophenone

**M. R. Rizal and S. W. Ng**

## 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.

## Experimental

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

## 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.

## Figures

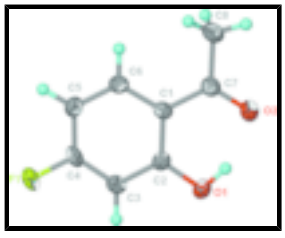

Fig. 1. 70% Probability thermal ellipsoid plot of 4'-fluoro-2'-hydroxyacetophenone. Hydrogen atoms are drawn as spheres of arbitrary radius.

## 4-fluoro-2-hydroxybenzaldehyde

*Crystal data*

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

$V$ = 703.27 (3) Å$^3$
$Z$ = 4

0.16 × 0.14 × 0.12 mm

*Data collection*

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
$T$ = 100(2) K
ω scans
Absorption correction: none
8762 measured reflections
1601 independent reflections

1224 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 27.5º
$\theta_{min}$ = 2.1º
$h$ = −4→4
$k$ = −18→18
$l$ = −16→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$^{-3}$
Extinction correction: none

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, °)*

| | | | |
|---|---|---|---|
| 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, °)*

| *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) |

**Fig. 1**