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## Structure Reports

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3-Fluoro-*N*-(*p*-tolyl)benzamideAamer Saeed,<sup>a\*</sup> Rasheed Ahmad Khera,<sup>a</sup> Kazuma Gotoh<sup>b</sup> and Hiroyuki Ishida<sup>b</sup><sup>a</sup>Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and <sup>b</sup>Department of Chemistry, Faculty of Science, Okayama University, Okayama 700-8530, Japan

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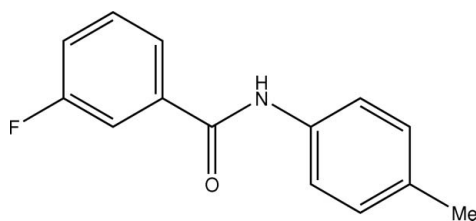
Received 17 September 2008; accepted 7 October 2008

Key indicators: single-crystal X-ray study;  $T = 223$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.073;  $wR$  factor = 0.240; data-to-parameter ratio = 21.2.

In the crystal structure of the title compound,  $\text{C}_{14}\text{H}_{12}\text{FNO}$ , the amide  $-\text{NHCO}-$  mean plane makes dihedral angles of 28.6 (2) and 37.5 (2)° with the mean planes through the fluorobenzene and methylbenzene units, respectively. The dihedral angle between the two benzene ring mean planes is 65.69 (10)°. In the crystal structure, molecules are linked through  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and stack along the  $b$  axis.

## Related literature

For related structures, see: Chopra & Row (2005); Saeed *et al.* (2008).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{12}\text{FNO}$  $M_r = 229.25$ 

Monoclinic,  $C2/c$   
 $a = 27.645$  (3) Å  
 $b = 5.2618$  (6) Å  
 $c = 15.892$  (2) Å  
 $\beta = 93.519$  (3)°  
 $V = 2307.3$  (5) Å<sup>3</sup>

$Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 223$  (1) K  
 $0.40 \times 0.35 \times 0.18$  mm

## Data collection

Rigaku R-Axis RAPIDII  
 diffractometer  
 Absorption correction: numerical  
 (ABSCOR; Higashi, 1999)  
 $T_{\min} = 0.968$ ,  $T_{\max} = 0.983$

13860 measured reflections  
 3357 independent reflections  
 1779 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.055$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.073$   
 $wR(F^2) = 0.240$   
 $S = 1.01$   
 3357 reflections  
 158 parameters

H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $\Delta\rho_{\max} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.21$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.77 (2)	2.35 (2)	3.087 (3)	161 (2)

Symmetry code: (i)  $x, y - 1, z$ .

Data collection: *PROCESS-AUTO* (Rigaku/MSK, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2064).

## References

- Chopra, D. & Row, T. N. G. (2005). *Cryst. Growth Des.* **5**, 1679–1681.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
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**supplementary materials**

*Acta Cryst.* (2008). E64, o2098 [ doi:10.1107/S160053680803225X ]

### 3-Fluoro-*N*-(*p*-tolyl)benzamide

A. Saeed, R. A. Khera, K. Gotoh and H. Ishida

#### Comment

The background to this study has been described in our earlier paper on 4-chloro-*N*-(2-chlorophenyl)-benzamide (Saeed *et al.*, 2008).

In the crystal structure of the title compound the two benzene rings are considerably twisted with respect to one another, with a dihedral angle of 65.69 (10)°. The amide –NHCO– mean plane makes dihedral angles of 28.6 (2) and 37.5 (2)° with the best mean planes through the fluorobenzene and methylbenzene units, respectively. In the crystal the molecules are linked through N—H···O hydrogen bonds and stack up the *b* axis.

No C—H···F hydrogen bonds were observed here, in contrast to the situation in 4-fluoro-*N*-(2-fluorophenyl)-benzamide (Chopra & Row, 2005).

#### Experimental

4-Fluorobenzoyl chloride (5.4 mmol) in CHCl<sub>3</sub> was treated with 4-methylaniline (21.6 mmol) under a nitrogen atmosphere at reflux for 4 h. Upon cooling the reaction mixture was diluted with CHCl<sub>3</sub> and washed consecutively with aq 1 M HCl and saturated aq NaHCO<sub>3</sub>. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. Crystallization of the residue in CHCl<sub>3</sub> afforded the title compound (84%) as white needles: Anal. calcd. for C<sub>14</sub>H<sub>12</sub>FNO: C 73.35, H 5.28, N 6.11%; found: C 73.30, H 5.32, N 6.09%.

#### Refinement

The N-bound H atom was located in a difference Fourier map and was freely refined. The other H atoms were positioned geometrically (C—H = 0.94 and 0.97 Å) and treated as riding atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

#### Figures

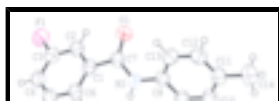


Fig. 1. A view of the molecular structure of the title compound. The displacement ellipsoids are drawn at the 40% probability level.



Fig. 2. A view along the *b* axis of the crystal packing of the title compound.

## 3-Fluoro-*N*-(*p*-tolyl)benzamide

### Crystal data

C<sub>14</sub>H<sub>12</sub>FNO

$M_r = 229.25$

Monoclinic, *C*2/*c*

Hall symbol: -*C* 2yc

$a = 27.645$  (3) Å

$b = 5.2618$  (6) Å

$c = 15.892$  (2) Å

$\beta = 93.519$  (3)°

$V = 2307.3$  (5) Å<sup>3</sup>

$Z = 8$

$F_{000} = 960.00$

$D_x = 1.320$  Mg m<sup>-3</sup>

Mo *K*α radiation

$\lambda = 0.71075$  Å

Cell parameters from 7127 reflections

$\theta = 3.0$ – $30.0$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 223$  (1) K

Block, colorless

$0.40 \times 0.35 \times 0.18$  mm

### Data collection

Rigaku R-AXIS RAPIDII  
diffractometer

Detector resolution: 10.00 pixels mm<sup>-1</sup>

$T = 223$ (2) K

$\omega$  scans

Absorption correction: numerical  
(*ABSCOR*; Higashi, 1999)

$T_{\min} = 0.968$ ,  $T_{\max} = 0.983$

13860 measured reflections

3357 independent reflections

1779 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\text{max}} = 30.0$ °

$h = -38$ → $38$

$k = -6$ → $7$

$l = -22$ → $22$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.073$

$wR(F^2) = 0.240$

$S = 1.01$

3357 reflections

158 parameters

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

H atoms treated by a mixture of  
independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1335P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.20$  e Å<sup>-3</sup>

Extinction correction: none

### 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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.69906 (5)	0.5995 (3)	0.23465 (10)	0.0965 (5)
O1	0.52251 (5)	0.6096 (3)	0.14071 (11)	0.0781 (5)
N1	0.50521 (6)	0.1882 (4)	0.12722 (11)	0.0639 (5)
C1	0.58887 (6)	0.3226 (4)	0.14164 (11)	0.0594 (5)
C2	0.62009 (7)	0.4878 (4)	0.18591 (12)	0.0656 (5)
H2	0.6081	0.6327	0.2122	0.079*
C3	0.66868 (8)	0.4361 (4)	0.19066 (14)	0.0703 (5)
C4	0.68819 (7)	0.2292 (5)	0.15293 (14)	0.0745 (6)
H4	0.7217	0.1984	0.1576	0.089*
C5	0.65712 (7)	0.0677 (4)	0.10794 (14)	0.0732 (6)
H5	0.6697	-0.0741	0.0807	0.088*
C6	0.60772 (7)	0.1105 (4)	0.10214 (12)	0.0657 (5)
H6	0.5869	-0.0026	0.0718	0.079*
C7	0.53603 (7)	0.3860 (4)	0.13667 (11)	0.0608 (5)
C8	0.45358 (7)	0.2026 (4)	0.11934 (11)	0.0599 (5)
C9	0.42706 (7)	0.0146 (4)	0.15561 (13)	0.0675 (5)
H9	0.4431	-0.1164	0.1865	0.081*
C10	0.37703 (7)	0.0181 (4)	0.14673 (13)	0.0729 (6)
H10	0.3594	-0.1125	0.1712	0.087*
C11	0.35222 (7)	0.2093 (4)	0.10264 (11)	0.0675 (5)
C12	0.37940 (7)	0.3956 (4)	0.06655 (13)	0.0705 (6)
H12	0.3634	0.5269	0.0359	0.085*
C13	0.42967 (8)	0.3940 (4)	0.07434 (13)	0.0704 (5)
H13	0.4474	0.5228	0.0491	0.085*
C14	0.29774 (8)	0.2111 (6)	0.09397 (16)	0.0916 (8)
H14A	0.2850	0.2043	0.1495	0.137*
H14B	0.2864	0.0647	0.0613	0.137*
H14C	0.2867	0.3655	0.0655	0.137*
H1	0.5158 (7)	0.055 (4)	0.1353 (12)	0.058 (6)*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0752 (8)	0.0995 (10)	0.1131 (11)	-0.0114 (7)	-0.0082 (7)	-0.0173 (8)
O1	0.0711 (9)	0.0616 (9)	0.1023 (12)	0.0027 (7)	0.0107 (7)	-0.0059 (7)
N1	0.0633 (9)	0.0566 (9)	0.0719 (10)	0.0009 (9)	0.0063 (7)	0.0030 (8)
C1	0.0655 (11)	0.0619 (10)	0.0518 (9)	-0.0016 (8)	0.0112 (7)	0.0049 (7)

## supplementary materials

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C2	0.0692 (12)	0.0646 (11)	0.0636 (11)	-0.0002 (10)	0.0087 (8)	-0.0013 (9)
C3	0.0681 (12)	0.0758 (13)	0.0669 (11)	-0.0049 (10)	0.0035 (9)	0.0027 (9)
C4	0.0648 (11)	0.0822 (14)	0.0779 (13)	0.0043 (11)	0.0148 (9)	0.0089 (11)
C5	0.0746 (13)	0.0759 (13)	0.0709 (12)	0.0088 (11)	0.0190 (9)	-0.0006 (10)
C6	0.0705 (11)	0.0665 (11)	0.0610 (10)	0.0004 (9)	0.0127 (8)	-0.0028 (8)
C7	0.0625 (10)	0.0636 (11)	0.0570 (10)	0.0008 (9)	0.0088 (8)	-0.0002 (8)
C8	0.0605 (10)	0.0645 (10)	0.0551 (9)	-0.0013 (8)	0.0076 (7)	-0.0050 (8)
C9	0.0657 (11)	0.0717 (12)	0.0659 (11)	0.0011 (9)	0.0100 (8)	0.0067 (9)
C10	0.0717 (12)	0.0787 (13)	0.0694 (12)	-0.0049 (11)	0.0141 (9)	0.0063 (10)
C11	0.0635 (11)	0.0852 (14)	0.0540 (10)	0.0019 (10)	0.0058 (8)	-0.0085 (9)
C12	0.0712 (12)	0.0729 (13)	0.0663 (12)	0.0063 (10)	-0.0044 (9)	0.0028 (9)
C13	0.0763 (12)	0.0725 (12)	0.0626 (11)	-0.0045 (10)	0.0041 (9)	0.0088 (9)
C14	0.0683 (13)	0.126 (2)	0.0807 (15)	0.0047 (14)	0.0050 (11)	-0.0041 (14)

### *Geometric parameters (Å, °)*

F1—C3	1.364 (2)	C6—H6	0.9400
O1—C7	1.238 (2)	C8—C9	1.378 (3)
N1—C7	1.347 (3)	C8—C13	1.380 (3)
N1—C8	1.427 (2)	C9—C10	1.382 (3)
N1—H1	0.77 (2)	C9—H9	0.9400
C1—C2	1.386 (3)	C10—C11	1.384 (3)
C1—C6	1.397 (3)	C10—H10	0.9400
C1—C7	1.496 (3)	C11—C12	1.381 (3)
C2—C3	1.368 (3)	C11—C14	1.504 (3)
C2—H2	0.9400	C12—C13	1.388 (3)
C3—C4	1.370 (3)	C12—H12	0.9400
C4—C5	1.377 (3)	C13—H13	0.9400
C4—H4	0.9400	C14—H14A	0.9700
C5—C6	1.382 (3)	C14—H14B	0.9700
C5—H5	0.9400	C14—H14C	0.9700
C7—N1—C8	126.25 (17)	C9—C8—C13	119.37 (18)
C7—N1—H1	117.0 (15)	C9—C8—N1	118.68 (17)
C8—N1—H1	115.6 (15)	C13—C8—N1	121.91 (17)
C2—C1—C6	119.43 (17)	C8—C9—C10	120.14 (19)
C2—C1—C7	117.56 (17)	C8—C9—H9	119.9
C6—C1—C7	122.99 (17)	C10—C9—H9	119.9
C3—C2—C1	118.83 (19)	C9—C10—C11	121.58 (19)
C3—C2—H2	120.6	C9—C10—H10	119.2
C1—C2—H2	120.6	C11—C10—H10	119.2
F1—C3—C2	118.34 (19)	C12—C11—C10	117.44 (17)
F1—C3—C4	118.61 (19)	C12—C11—C14	121.6 (2)
C2—C3—C4	123.05 (19)	C10—C11—C14	120.9 (2)
C3—C4—C5	117.92 (19)	C11—C12—C13	121.75 (18)
C3—C4—H4	121.0	C11—C12—H12	119.1
C5—C4—H4	121.0	C13—C12—H12	119.1
C4—C5—C6	121.1 (2)	C8—C13—C12	119.71 (18)
C4—C5—H5	119.4	C8—C13—H13	120.1
C6—C5—H5	119.4	C12—C13—H13	120.1

C5—C6—C1	119.65 (19)	C11—C14—H14A	109.5
C5—C6—H6	120.2	C11—C14—H14B	109.5
C1—C6—H6	120.2	H14A—C14—H14B	109.5
O1—C7—N1	123.30 (18)	C11—C14—H14C	109.5
O1—C7—C1	120.43 (17)	H14A—C14—H14C	109.5
N1—C7—C1	116.27 (17)	H14B—C14—H14C	109.5
C6—C1—C2—C3	-0.9 (3)	C2—C1—C7—N1	-152.62 (17)
C7—C1—C2—C3	-179.24 (17)	C6—C1—C7—N1	29.1 (3)
C1—C2—C3—F1	-179.77 (18)	C7—N1—C8—C9	-144.0 (2)
C1—C2—C3—C4	0.6 (3)	C7—N1—C8—C13	38.1 (3)
F1—C3—C4—C5	-179.27 (19)	C13—C8—C9—C10	0.1 (3)
C2—C3—C4—C5	0.3 (3)	N1—C8—C9—C10	-177.82 (17)
C3—C4—C5—C6	-1.0 (3)	C8—C9—C10—C11	-0.8 (3)
C4—C5—C6—C1	0.8 (3)	C9—C10—C11—C12	0.9 (3)
C2—C1—C6—C5	0.2 (3)	C9—C10—C11—C14	-179.65 (19)
C7—C1—C6—C5	178.47 (18)	C10—C11—C12—C13	-0.5 (3)
C8—N1—C7—O1	0.9 (3)	C14—C11—C12—C13	-179.9 (2)
C8—N1—C7—C1	-178.66 (15)	C9—C8—C13—C12	0.3 (3)
C2—C1—C7—O1	27.8 (3)	N1—C8—C13—C12	178.19 (17)
C6—C1—C7—O1	-150.5 (2)	C11—C12—C13—C8	-0.1 (3)

*Hydrogen-bond geometry* (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O1 <sup>i</sup>	0.77 (2)	2.35 (2)	3.087 (3)	161 (2)

Symmetry codes: (i) *x*, *y*-1, *z*.

Fig. 1

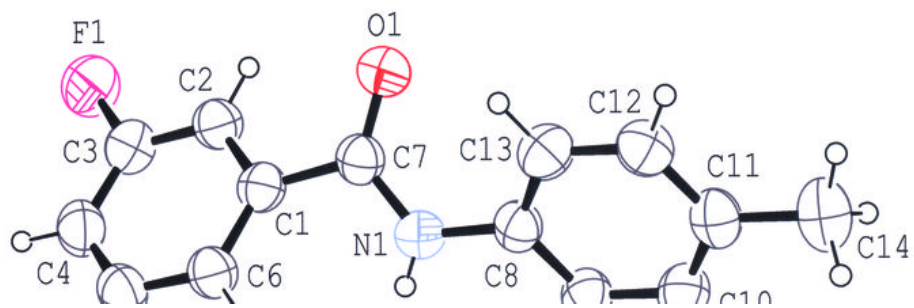


Fig. 2

