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3-(2-Fluorophenyl)-2-phenylacrylic acid

Tariq Mahmood Babar,[a] Nasim Hasan Rama,[a]* Ghulam Qadeer,[a] Gul Shahzada Khan[a] and Wai-Yeung Wong[b]

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]Department of Chemistry, Hong Kong Baptist University, Waterloo Road, Kowloon Tong, Hong Kong

Correspondence e-mail: nasim_hasan_rama@hotmail.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 13.0

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

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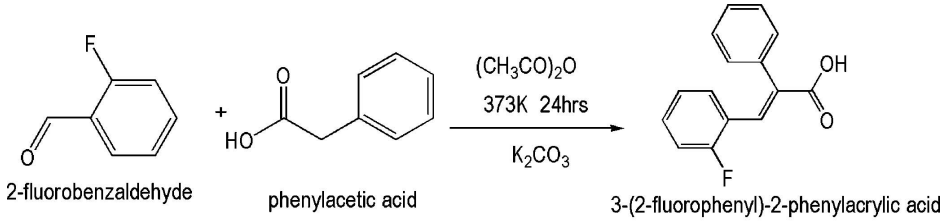
The title compound, $C_{15}H_{11}FO_2$, is a derivative of α-phenylcinnamic acid. The two benzene rings in the molecule are approximately perpendicular to each other. O—H···O hydrogen bonding occurs between molecules.

Comment

Cinnamic acid derivatives are important building blocks in the production of lignins in higher plants (Mann, 1987). They are also key intermediates used in shikimic acid metabolic pathways of higher plants (Forgo *et al.*, 2005). They are widely used as the starting materials for the synthesis of antimalarial drugs. The presence of the fluorine group shows an increase in the effectiveness of these compounds in prototype medicinals (Noddif *et al.*, 1971). In these acids, the main structural feature is the strong hydrogen bonding between the carbonyl O atom of one molecule and H atom of another, which is responsible for the formation and stabilization of the dimer. In view of the importance of this class of compounds, the title compound, (I), has been synthesized, and its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The bond lengths within the benzene rings range from 1.364 (4) Å to 1.397 (3) Å, typical of aromatic character. The C2—C1—C6 bond angle of 124.0 (2)° shows a small deviation from the ideal value of 120°. The bond length of 1.336 (2) Å shows C7═C8 to have double-bond character. Owing to the electronegative nature of fluorine, the C1—F1 bond length of 1.353 (2) Å is shorter than a normal single bond length (1.39 Å).

Strong intermolecular hydrogen bonding is found between carboxyl groups in the crystal structure of (I) (Table 1).

Experimental

The acid was synthesized according to a reported procedure (Noddif *et al.*, 1971). A mixture of phenylacetic acid (4.08 g, 30 mmol), 2-fluorobenzaldehyde (3.13 ml, 30 mmol), potassium carbonate (2.346 g, 17 mmol) and acetic anhydride (7.07 ml, 75 mmol) were

heated (see scheme). The temperature was slowly raised to 373 K and maintained for 24 h. Water (400 ml) and hydrochloric acid (200 ml, 10%) were added, and the reaction mixture was stirred at room temperature for 2 h and then filtered. The precipitate was washed with water (100 ml × 3) to remove the impurities (yield 86%). Colourless single crystals of (I) were obtained from an ethyl acetate solution.

Crystal data

$C_{15}H_{11}FO_2$
M_r = 242.24
Monoclinic, $P2_1/c$
a = 9.1942 (8) Å
b = 5.7823 (5) Å
c = 23.126 (2) Å
β = 96.398 (2)°
V = 1221.78 (18) Å^3
Z = 4
D_x = 1.317 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Rod, colourless
0.30 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.765, T_{max} = 0.990
5802 measured reflections
2181 independent reflections
1830 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.121
S = 1.04
2181 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.3354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.020 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	1.02 (3)	1.64 (3)	2.6579 (17)	177 (3)

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

The carboxyl H atom was located in a difference Fourier map and refined isotropically. Other H atoms were placed in calculated positions with C—H = 0.93 Å, and refined in riding mode; U_{iso}(H) = 1.2U_{eq}(C).

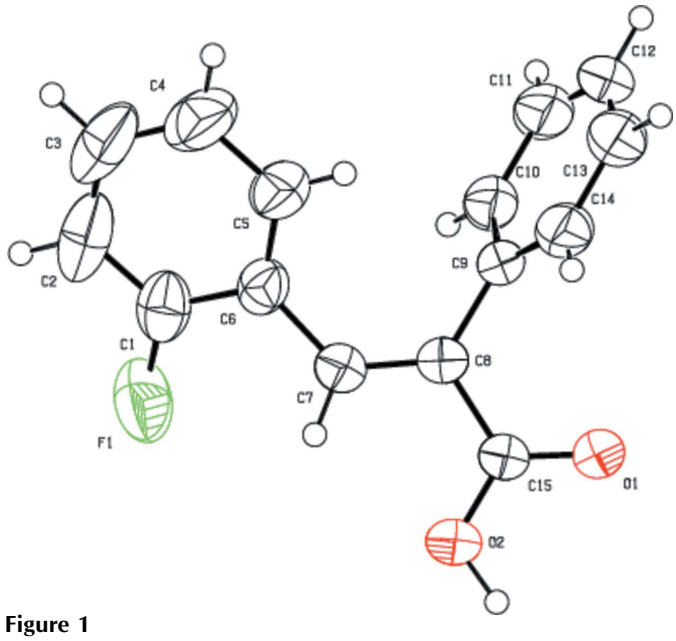


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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