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3-(2-Furyl)-1-(4-nitrophenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.070
wR factor = 0.198
Data-to-parameter ratio = 35.2

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

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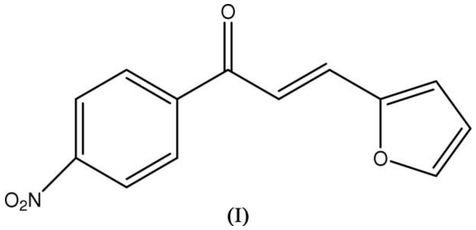
In the title compound, $C_{13}H_9NO_4$, the dihedral angle between the benzene and furan rings is 6.23 (5)°. The crystal structure is stabilized by weak intermolecular C—H···O hydrogen bonds.

Comment

Chalcones show interesting biological and pharmacological activities (De Vincenzo *et al.*, 1995; Kumar *et al.*, 2003). In addition, chalcones with appropriate subtituents constitute a class of non-linear optical materials (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991, Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000). In this paper, we present the crystal structure of the title compound, (I), which does not exhibit second-order non-linear optical properties as it crystallizes out in a centrosymmetric space group.



(I)

In (I) (Fig. 1), the bond lengths and angles have normal values (Allen *et al.*, 1987), comparable with those found in related structures (Teh *et al.*, 2006; Patil *et al.*, 2006*a*,*b*; Ng *et al.*, 2006; Rosli *et al.*, 2006). The least-squares plane through the enone group makes dihedral angles of 4.19 (5) and 2.14 (6)°, respectively, with the benzene and furan rings. The dihedral angle between the two rings is 6.23 (5)°. The nitro group at C3 is almost coplanar with the C1–C6 benzene ring, with O4—N1—C3—C4 and O3—N1—C3—C2 torsion angles of −3.49 (19) and −4.38 (18)°, respectively.

The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

Chalcone derivative (I) was obtained by the condensation of 2-furfuraldehyde (0.01 mol) with 4-nitroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (2 ml, 30%). After stirring for 2 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand for 24 h. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. The purity of the compound was checked by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction experiments were grown in 8 d by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{13}H_9NO_4$
$M_r = 243.21$
Monoclinic, $P2_1/c$
$a = 3.8809$ (2) Å
$b = 10.6603$ (4) Å
$c = 26.5500$ (11) Å
$\beta = 94.867$ (3)°
$V = 1094.45$ (8) Å^3
$Z = 4$
$D_x = 1.476$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 100.0$ (1) K
Plate, yellow
0.54 × 0.38 × 0.10 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.806$, $T_{\max} = 0.989$
28259 measured reflections
5741 independent reflections
3956 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.067$
$\theta_{\max} = 37.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.198$
$S = 1.10$
5741 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2 + 0.1328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.56$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O2$^{\rm i}$	0.93	2.48	3.151 (2)	129
C12—H12A···O3$^{\rm ii}$	0.93	2.55	3.463 (2)	169

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

H atoms were placed in calculated positions, with C—H distances of 0.93 Å, and treated as riding. The $U_{\rm iso}$(H) values were constrained to be $1.2U_{\rm eq}$(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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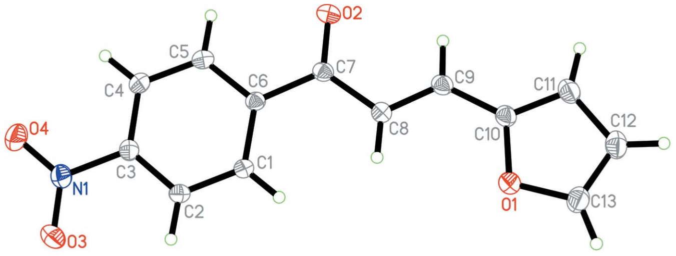

Figure 1
View of (I), showing the atomic numbering and 50% probability displacement ellipsoids.

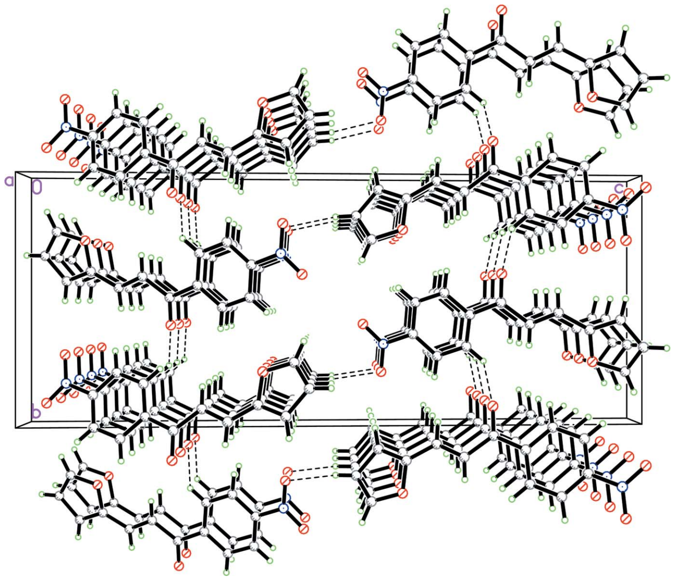

Figure 2
The crystal packing, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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o2398 Patil *et al.* • $C_{13}H_9NO_4$ *Acta Cryst.* (2006). E**62**, o2397–o2398