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

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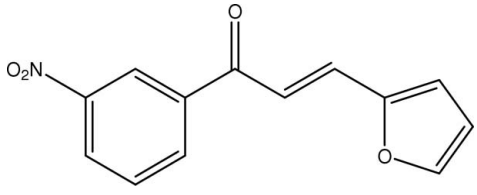
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.119; data-to-parameter ratio = 19.5.

In the title compound, $C_{13}H_9NO_4$, the dihedral angle between the benzene and furan rings is 31.63 (6)°. The nitro group is almost coplanar with the attached benzene ring. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules, forming chains along the b axis.

Related literature

For bond length data, see: Allen *et al.* (1987). For hydrogen bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Patil, Dharmaprakash *et al.* (2006); Patil, Teh *et al.* (2006); Patil, Dharmaprakash *et al.* (2007); Patil, Teh *et al.* (2007); Kiran *et al.* (2007).



Experimental

Crystal data

$C_{13}H_9NO_4$
M_r = 243.21
Monoclinic, $P2_1/c$
a = 6.2162 (1) Å
b = 26.6985 (5) Å
c = 7.0467 (2) Å
β = 111.625 (1)°
V = 1087.18 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100.0 (1) K
0.54 × 0.48 × 0.25 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.867, T_{max} = 0.973
18132 measured reflections
3171 independent reflections
2843 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.119
S = 1.04
3171 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O2	0.93	2.48	2.807 (1)	101
C1—H1A···O4^{i}	0.93	2.36	3.073 (2)	133

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

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* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2371).

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supplementary materials

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

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Comment

Many chalcone derivatives exhibit non-linear optical properties (Patil, Dharmaprakash *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2007; Patil, Teh *et al.*, 2007; John Kiran *et al.*, 2007). We report here the structure of the title compound, (I) (Fig. 1), which crystallizes in a centrosymmetric space group and this precludes second-order non-linear optical properties.

Bond lengths and angles in (I) display normal values (Allen *et al.*, 1987), comparable to those of a related structure (Patil, Teh *et al.*, 2006). The molecule is slightly twisted about the C7—C8 bond; the diheral angle between the benzene (C8—C13) and furan (O1/C1-4) rings is 31.63 (6)°. The nitro group at C10 is almost coplanar with the attached benzene ring, with a O3—N1—C10—C9 torsion angle of 4.42 (15)°.

An intramolecular C5—H5A···O2 hydrogen bond (Table 1 and Figure 1) generates an S(5) ring motif (Bernstein *et al.*, 1995). In the crystal structure, the molecules are linked by intermolecular C1—H1A···O4^{i} interactions (Table 1) into infinite chains along the *b* axis (Fig. 2).

Experimental

An aqueous solution of sodium hydroxide (5%, 5 ml) was added with stirring (2 h) to a solution of 2-furfuraldehyde (0.01 mol) and 3-nitroacetophenone (0.01 mol) in methanol (60 ml) at room temperature. The reaction mixture was then poured on to ice-cold water. The precipitate that formed was filtered off, dried and recrystallized from acetone. Crystals suitable for single-crystal X-ray diffraction experiments were grown by slow evaporation of an acetone solution at room temperature.

Refinement

H atoms were placed in calculated positions and constrained to ride on their carrier atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

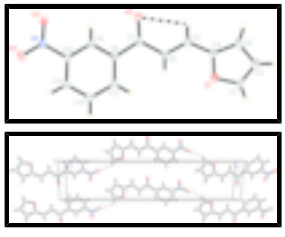

Figure 1 The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates a hydrogen bond.

Figure 2 The crystal packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

3-(2-furyl)-1-(3-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{13}H_9NO_4$	F_{000} = 504
M_r = 243.21	D_x = 1.486 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7407 reflections
a = 6.2162 (1) Å	θ = 3.1–30.0º
b = 26.6985 (5) Å	μ = 0.11 mm^{-1}
c = 7.0467 (2) Å	T = 100.0 (1) K
β = 111.625 (1)º	Block, colourless
V = 1087.18 (4) Å^3	0.54 × 0.48 × 0.25 mm
Z = 4	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	3171 independent reflections
Radiation source: fine-focus sealed tube	2843 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.0º
T = 100.0(1) K	θ_{min} = 3.1º
ω scans	h = −8→8
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −37→37
T_{min} = 0.867, T_{max} = 0.973	l = −9→6
18132 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.4848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.119	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
3171 reflections	Extinction correction: none
163 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.07026 (15)	−0.15417 (3)	0.84028 (14)	0.0257 (2)
O2	0.57685 (14)	−0.01469 (3)	0.74585 (14)	0.02326 (19)
O3	0.47514 (17)	0.15705 (3)	0.49383 (16)	0.0291 (2)
O4	0.23696 (16)	0.20552 (3)	0.56597 (15)	0.0274 (2)
N1	0.31969 (17)	0.16410 (3)	0.55825 (15)	0.0202 (2)
C1	0.0349 (2)	−0.20133 (5)	0.8965 (2)	0.0295 (3)
H1A	−0.1086	−0.2142	0.8848	0.035*
C2	0.2345 (3)	−0.22679 (4)	0.97100 (19)	0.0286 (3)
H2A	0.2546	−0.2594	1.0205	0.034*
C3	0.4109 (2)	−0.19372 (4)	0.95922 (19)	0.0261 (3)
H3A	0.5677	−0.2008	0.9981	0.031*
C4	0.30335 (19)	−0.14976 (4)	0.87972 (17)	0.0190 (2)
C5	0.39115 (19)	−0.10293 (4)	0.83949 (16)	0.0193 (2)
H5A	0.5476	−0.1014	0.8598	0.023*
C6	0.26585 (19)	−0.06104 (4)	0.77482 (17)	0.0196 (2)
H6A	0.1081	−0.0612	0.7498	0.024*
C7	0.37869 (18)	−0.01487 (4)	0.74362 (16)	0.0178 (2)
C8	0.24853 (17)	0.03362 (4)	0.71599 (16)	0.0166 (2)
C9	0.33063 (17)	0.07452 (4)	0.63862 (16)	0.0163 (2)
H9A	0.4520	0.0707	0.5926	0.020*
C10	0.22716 (18)	0.12077 (4)	0.63202 (16)	0.0172 (2)
C11	0.04387 (19)	0.12809 (4)	0.69681 (18)	0.0206 (2)
H11A	−0.0214	0.1596	0.6918	0.025*
C12	−0.03893 (19)	0.08711 (5)	0.76911 (18)	0.0223 (2)
H12A	−0.1627	0.0910	0.8119	0.027*
C13	0.06153 (18)	0.04004 (4)	0.77829 (17)	0.0199 (2)
H13A	0.0036	0.0127	0.8262	0.024*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0266 (4)	0.0177 (4)	0.0336 (5)	−0.0053 (3)	0.0119 (4)	0.0002 (3)
O2	0.0215 (4)	0.0196 (4)	0.0307 (4)	−0.0001 (3)	0.0119 (3)	0.0027 (3)
O3	0.0332 (5)	0.0201 (4)	0.0434 (5)	0.0002 (3)	0.0251 (4)	0.0029 (4)
O4	0.0322 (5)	0.0142 (4)	0.0361 (5)	0.0035 (3)	0.0130 (4)	−0.0011 (3)
N1	0.0226 (4)	0.0147 (4)	0.0233 (5)	−0.0002 (3)	0.0082 (4)	−0.0003 (3)
C1	0.0397 (7)	0.0187 (5)	0.0345 (7)	−0.0093 (5)	0.0188 (6)	−0.0014 (4)
C2	0.0466 (7)	0.0166 (5)	0.0233 (5)	−0.0043 (5)	0.0136 (5)	−0.0004 (4)
C3	0.0334 (6)	0.0188 (5)	0.0241 (5)	0.0034 (4)	0.0083 (5)	−0.0020 (4)
C4	0.0226 (5)	0.0164 (5)	0.0180 (5)	−0.0024 (4)	0.0074 (4)	−0.0016 (4)
C5	0.0229 (5)	0.0172 (5)	0.0171 (5)	−0.0040 (4)	0.0066 (4)	−0.0020 (4)
C6	0.0199 (5)	0.0176 (5)	0.0194 (5)	−0.0046 (4)	0.0049 (4)	0.0001 (4)
C7	0.0200 (5)	0.0158 (4)	0.0164 (5)	−0.0025 (4)	0.0052 (4)	0.0001 (3)
C8	0.0162 (4)	0.0161 (4)	0.0161 (4)	−0.0023 (3)	0.0045 (3)	−0.0007 (3)
C9	0.0161 (4)	0.0154 (4)	0.0177 (4)	−0.0013 (3)	0.0065 (4)	−0.0014 (3)
C10	0.0178 (4)	0.0149 (4)	0.0186 (5)	−0.0012 (3)	0.0063 (4)	−0.0008 (3)
C11	0.0187 (5)	0.0203 (5)	0.0221 (5)	0.0023 (4)	0.0069 (4)	−0.0024 (4)
C12	0.0170 (4)	0.0285 (6)	0.0231 (5)	−0.0005 (4)	0.0094 (4)	−0.0023 (4)
C13	0.0181 (4)	0.0228 (5)	0.0188 (5)	−0.0041 (4)	0.0069 (4)	−0.0002 (4)

Geometric parameters (Å, °)

O1—C1	1.3618 (14)	C5—H5A	0.93
O1—C4	1.3761 (14)	C6—C7	1.4744 (14)
O2—C7	1.2261 (13)	C6—H6A	0.93
O3—N1	1.2242 (13)	C7—C8	1.5008 (15)
O4—N1	1.2291 (12)	C8—C13	1.3963 (15)
N1—C10	1.4695 (14)	C8—C9	1.3982 (14)
C1—C2	1.341 (2)	C9—C10	1.3853 (14)
C1—H1A	0.93	C9—H9A	0.93
C2—C3	1.4335 (18)	C10—C11	1.3886 (15)
C2—H2A	0.93	C11—C12	1.3838 (16)
C3—C4	1.3646 (16)	C11—H11A	0.93
C3—H3A	0.93	C12—C13	1.3940 (16)
C4—C5	1.4338 (15)	C12—H12A	0.93
C5—C6	1.3430 (15)	C13—H13A	0.93
C1—O1—C4	106.94 (10)	O2—C7—C6	122.16 (10)
O3—N1—O4	123.71 (10)	O2—C7—C8	119.30 (9)
O3—N1—C10	118.40 (9)	C6—C7—C8	118.50 (9)
O4—N1—C10	117.89 (9)	C13—C8—C9	119.51 (10)
C2—C1—O1	110.92 (11)	C13—C8—C7	122.46 (10)
C2—C1—H1A	124.5	C9—C8—C7	117.87 (9)
O1—C1—H1A	124.5	C10—C9—C8	118.53 (10)
C1—C2—C3	106.41 (11)	C10—C9—H9A	120.7
C1—C2—H2A	126.8	C8—C9—H9A	120.7
C3—C2—H2A	126.8	C9—C10—C11	122.78 (10)
C4—C3—C2	106.51 (11)	C9—C10—N1	118.44 (9)
C4—C3—H3A	126.7	C11—C10—N1	118.76 (9)
C2—C3—H3A	126.7	C12—C11—C10	118.12 (10)
C3—C4—O1	109.22 (10)	C12—C11—H11A	120.9

C3—C4—C5	131.82 (11)	C10—C11—H11A	120.9
O1—C4—C5	118.94 (10)	C11—C12—C13	120.58 (10)
C6—C5—C4	125.31 (10)	C11—C12—H12A	119.7
C6—C5—H5A	117.3	C13—C12—H12A	119.7
C4—C5—H5A	117.3	C12—C13—C8	120.45 (10)
C5—C6—C7	119.91 (10)	C12—C13—H13A	119.8
C5—C6—H6A	120.0	C8—C13—H13A	119.8
C7—C6—H6A	120.0		
C4—O1—C1—C2	0.47 (15)	C6—C7—C8—C9	−164.92 (10)
O1—C1—C2—C3	−0.80 (15)	C13—C8—C9—C10	1.92 (15)
C1—C2—C3—C4	0.82 (14)	C7—C8—C9—C10	−173.42 (9)
C2—C3—C4—O1	−0.55 (13)	C8—C9—C10—C11	−0.74 (16)
C2—C3—C4—C5	177.65 (12)	C8—C9—C10—N1	177.61 (9)
C1—O1—C4—C3	0.07 (13)	O3—N1—C10—C9	4.42 (15)
C1—O1—C4—C5	−178.39 (10)	O4—N1—C10—C9	−175.18 (10)
C3—C4—C5—C6	−174.41 (12)	O3—N1—C10—C11	−177.16 (10)
O1—C4—C5—C6	3.64 (17)	O4—N1—C10—C11	3.24 (15)
C4—C5—C6—C7	178.59 (10)	C9—C10—C11—C12	−0.58 (17)
C5—C6—C7—O2	10.81 (17)	N1—C10—C11—C12	−178.93 (10)
C5—C6—C7—C8	−166.91 (10)	C10—C11—C12—C13	0.72 (17)
O2—C7—C8—C13	−157.90 (11)	C11—C12—C13—C8	0.47 (17)
C6—C7—C8—C13	19.89 (15)	C9—C8—C13—C12	−1.81 (16)
O2—C7—C8—C9	17.30 (15)	C7—C8—C13—C12	173.30 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···O2	0.93	2.48	2.807 (1)	101
C1—H1A···O4^{i}	0.93	2.36	3.073 (2)	133

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2.

Fig. 1

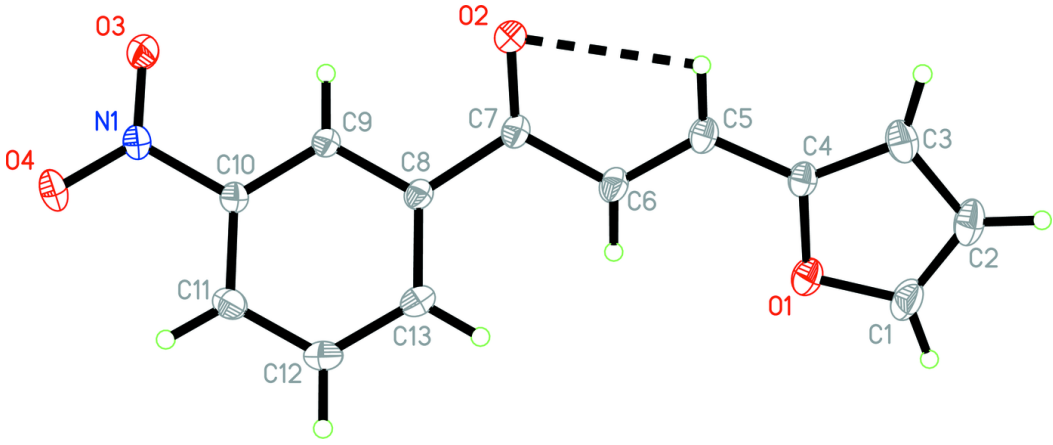

Fig. 2