Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-3-(4-Chlorophenyl)-1-(2-furyl)prop-2-en-1-one

Hoong-Kun Fun,[a]* P. S. Patil,[b] Samuel Robinson Jebas[a]‡ and S. M. Dharmaprakash[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India
Correspondence e-mail: hkfun@usm.my

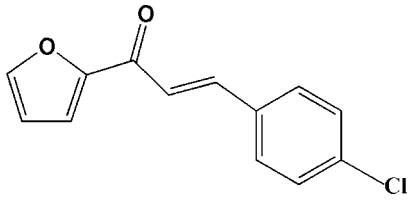
Received 2 July 2008; accepted 14 July 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 35.9.

In the title molecule, $C_{13}H_9ClO_2$, the benzene and furyl rings are slightly twisted from each other with a dihedral angle of 5.1 (1)°. An intramolecular C—H···O hydrogen-bond interaction generates an S(5) ring motif. In the crystal structure, molecules are stacked along the b axis and the crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds.

Related literature

For related literature on the biological and nonlinear optical properties of chalcone derivatives, see: Agrinskaya *et al.* (1999); Chopra *et al.* (2007); DiCesare & Lakowicz (2000); Patil *et al.* (2006, 2007); Gu, Ji, Patil & Dharmaprakash (2008); Gu, Ji, Patil, Dharmaprakash & Wang (2008). For bond-length data, see: Allen *et al.* (1987). For graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_9ClO_2$
M_r = 232.65
Orthorhombic, $Pna2_1$
a = 21.3399 (7) Å
b = 3.7912 (1) Å
c = 12.9444 (4) Å
V = 1047.25 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 100.0 (1) K
0.40 × 0.29 × 0.21 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.875, T_{max} = 0.931
13568 measured reflections
5209 independent reflections
4211 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.126
S = 1.08
5209 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 2227 Friedel pairs
Flack parameter: 0.07 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O2	0.93	2.52	2.8411 (17)	101
C13—H13A···O2^{i}	0.93	2.48	3.2535 (18)	140

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

HKF and SRJ thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. SRJ thanks the Universiti Sains Malaysia for a postdoctoral research fellowship. This work was supported by the Department of Science and Technology (DST), Government of India (grant No. SR/S2/LOP-17/2006).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2657).

References

Agrinskaya, N. V., Lukoshkin, V. A., Kudryavtsev, V. V., Nosova, G. I., Solovskaya, N. A. & Yakimanski, A. V. (1999). *Phys. Solid State*, **41**, 1914–1917.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chopra, D., Mohan, T. P., Vishalakshi, B. & Guru Row, T. N. (2007). *Acta Cryst.* C**63**, o704–o710.
DiCesare, N. & Lakowicz, J. R. (2000). *Tetrahedron Lett.* **43**, 2615–2618.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gu, B., Ji, W., Patil, P. S. & Dharmaprakash, S. M. (2008). *J. Appl. Phys.* **103**, 103511.
Gu, B., Ji, W., Patil, P. S., Dharmaprakash, S. M. & Wang, H. T. (2008). *Appl. Phys. Lett.* **92**, 091118.
Patil, P. S., Dharmaprakash, S. M., Fun, H.-K. & Karthikeyan, M. S. (2006). *J. Cryst. Growth*, **297**, 111–116.
Patil, P. S., Dharmaprakash, S. M., Ramakrishna, K., Fun, H.-K., Sai Santosh Kumar, R. & Rao, D. N. (2007). *J. Cryst. Growth*, **303**, 520–524.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

‡ Permanent address: Department of Physics, Karunya University, Karunya Nagar, Coimbatore 641 114, India.

supporting information

Acta Cryst. (2008). E**64**, o1530 [doi:10.1107/S1600536808021934]

(*E*)-3-(4-Chlorophenyl)-1-(2-furyl)prop-2-en-1-one

Hoong-Kun Fun, P. S. Patil, Samuel Robinson Jebas and S. M. Dharmaprakash

S1. Comment

Chalcone derivatives continue to attract the interest of chemists, biologists and physicists due to their remarkable biological and nonlinear optical properties (Chopra *et al.*, 2007; DiCesare & Lakowicz, 2000; Patil, *et al.*, 2006, 2007; Agrinskaya *et al.*, 1999; Gu, Ji, Patil & Dharmaprakash, 2008; Gu, Ji, Patil, Dharmaprakash & Wang, 2008). We have synthesized the title compound (I) and its structure is reported here.

The bond lengths and bond angles in (I) have normal values (Allen *et al.*, 1987). The benzene and furyl rings in the molecule are essentially planar with the maximum deviation from planarity being -0.003 (18)Å for atom C12 and -0.004 (14)Å for atom O1 respectively. The dihedral angle between the benzene and the furyl rings is 5.1 (1)°, indicating that they are only slightly twisted from each other.

An intramolecular C—H···O hydrogen bond generates an S(5) ring motif (Bernstein *et al.*, 1995). In the crystal structure, the molecules are are stacked along the *b* axis. The crystal packing is consolidated by C—H···O hydrogen bond interactions.

S2. Experimental

The compound (I) was synthesized by the condensation of 4 -chlorobenzaldehyde (0.01 mol, 1.49 g m) with 2-acetylfuran (0.01 mol, 1.01 ml) in methanol (60 ml) in the presence of a catalytic amount of sodium hydroxide solution (5 ml, 30%). After stirring (6 h), the contents of the flask were poured into ice-cold water (500 ml) and left to stand for 5 h. The resulting crude solid was filtered and dried. Then precipitated compound was recrystallized from N, *N*-dimethyl-formamide (DMF).

S3. Refinement

H atoms were positioned geometrically [C—H = 0.93 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

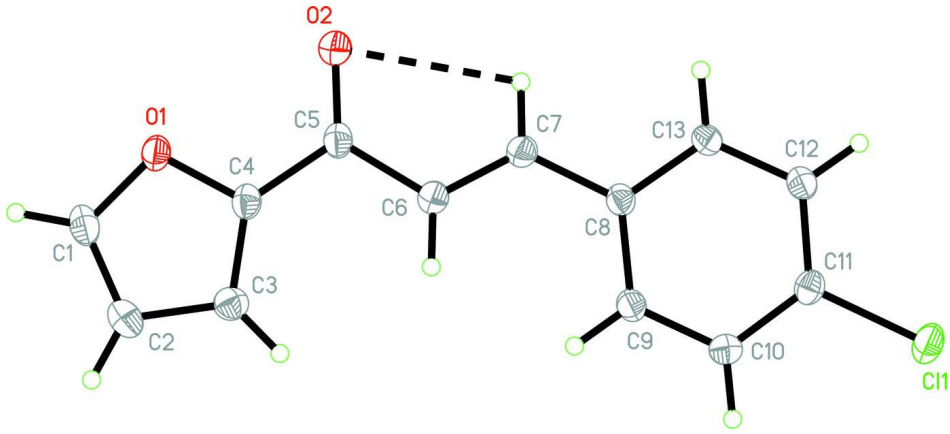


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme. The dashed line indicates a hydrogen bond.

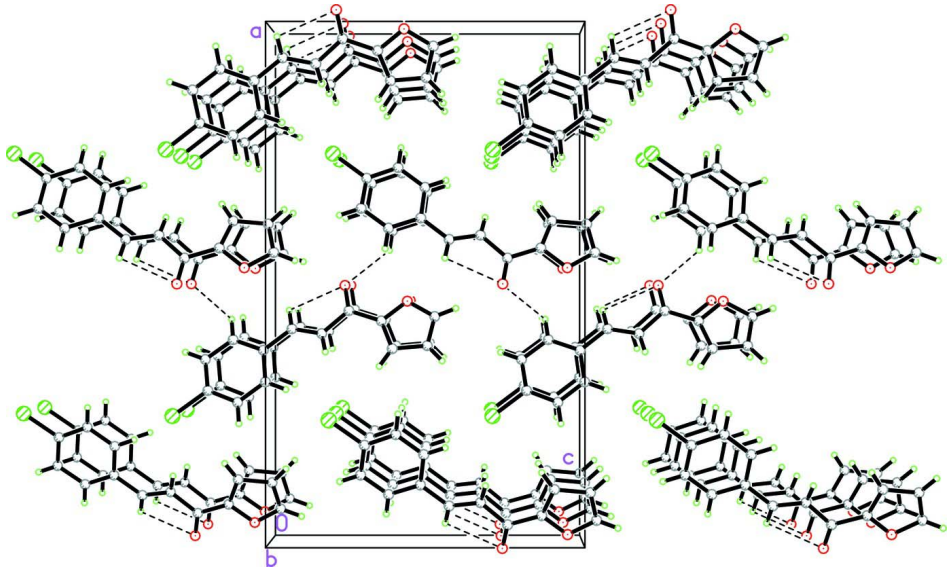


Figure 2

The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

(E)-3-(4-Chlorophenyl)-1-(2-furyl)prop-2-en-1-one

Crystal data

$C_{13}H_9ClO_2$
$M_r = 232.65$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 21.3399\ (7)$ Å
$b = 3.7912\ (1)$ Å
$c = 12.9444\ (4)$ Å
$V = 1047.25\ (5)$ Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.476$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4886 reflections
$\theta = 2.5–37.2°$
$\mu = 0.34$ mm^{-1}
$T = 100$ K
Block, colourless
0.40 × 0.29 × 0.21 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.875, T_{max} = 0.931
13568 measured reflections
5209 independent reflections
4211 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 38.2°, θ_{min} = 2.5°
h = −31→37
k = −6→6
l = −22→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.126
S = 1.08
5209 reflections
145 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 2216 Friedel pairs
Absolute structure parameter: 0.07 (6)

Special details

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

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.249271 (17)	0.53749 (9)	0.21078 (5)	0.02637 (9)
O1	0.03179 (5)	0.2805 (3)	0.94149 (7)	0.0225 (2)
O2	0.00152 (6)	0.1062 (3)	0.74067 (9)	0.0266 (2)
C1	0.06091 (7)	0.3896 (4)	1.02879 (11)	0.0246 (3)
H1A	0.0454	0.3557	1.0952	0.030*
C2	0.11562 (8)	0.5548 (4)	1.00653 (12)	0.0243 (3)
H2A	0.1437	0.6536	1.0533	0.029*
C3	0.12135 (7)	0.5463 (4)	0.89712 (12)	0.0215 (3)
H3A	0.1540	0.6388	0.8581	0.026*
C4	0.06937 (7)	0.3752 (4)	0.86037 (10)	0.0192 (2)
C5	0.04991 (6)	0.2723 (4)	0.75621 (9)	0.0198 (2)
C6	0.09349 (7)	0.3737 (4)	0.67253 (10)	0.0202 (2)
H6A	0.1274	0.5190	0.6875	0.024*
C7	0.08493 (6)	0.2600 (4)	0.57564 (10)	0.0188 (2)

H7A	0.0496	0.1223	0.5633	0.023*
C8	0.12568 (6)	0.3314 (4)	0.48732 (9)	0.0178 (2)
C9	0.18485 (6)	0.4918 (4)	0.49906 (11)	0.0188 (2)
H9A	0.1984	0.5579	0.5645	0.023*
C10	0.22299 (7)	0.5524 (4)	0.41438 (11)	0.0192 (2)
H10A	0.2621	0.6577	0.4223	0.023*
C11	0.20160 (7)	0.4524 (4)	0.31741 (11)	0.0186 (2)
C12	0.14356 (7)	0.2960 (4)	0.30286 (10)	0.0198 (2)
H12A	0.1301	0.2333	0.2370	0.024*
C13	0.10594 (6)	0.2350 (4)	0.38834 (9)	0.0185 (2)
H13A	0.0670	0.1284	0.3797	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02847 (16)	0.02869 (17)	0.02196 (14)	−0.00201 (13)	0.00812 (11)	0.00173 (17)
O1	0.0200 (4)	0.0321 (6)	0.0156 (4)	0.0000 (4)	0.0017 (3)	0.0021 (4)
O2	0.0241 (5)	0.0361 (6)	0.0196 (4)	−0.0065 (4)	0.0001 (4)	0.0017 (4)
C1	0.0265 (7)	0.0314 (8)	0.0161 (5)	0.0055 (6)	−0.0005 (5)	−0.0023 (5)
C2	0.0268 (7)	0.0249 (7)	0.0211 (6)	0.0033 (5)	−0.0045 (5)	−0.0027 (5)
C3	0.0201 (6)	0.0220 (7)	0.0223 (6)	0.0000 (5)	−0.0018 (5)	0.0026 (5)
C4	0.0201 (5)	0.0218 (6)	0.0157 (5)	0.0029 (5)	0.0008 (4)	0.0019 (4)
C5	0.0204 (6)	0.0236 (6)	0.0153 (5)	0.0028 (5)	0.0010 (4)	0.0013 (4)
C6	0.0196 (5)	0.0224 (6)	0.0185 (5)	−0.0008 (5)	0.0010 (4)	0.0006 (5)
C7	0.0186 (5)	0.0197 (6)	0.0181 (5)	−0.0006 (5)	0.0004 (4)	0.0011 (4)
C8	0.0171 (5)	0.0209 (6)	0.0153 (5)	0.0020 (5)	−0.0006 (4)	−0.0002 (4)
C9	0.0191 (5)	0.0212 (6)	0.0160 (5)	0.0004 (5)	−0.0007 (4)	−0.0011 (4)
C10	0.0181 (6)	0.0187 (6)	0.0208 (5)	−0.0012 (5)	−0.0005 (4)	0.0003 (5)
C11	0.0209 (6)	0.0166 (6)	0.0185 (5)	0.0013 (5)	0.0031 (4)	0.0016 (4)
C12	0.0217 (6)	0.0212 (6)	0.0164 (5)	−0.0006 (5)	−0.0006 (4)	−0.0014 (4)
C13	0.0173 (5)	0.0218 (6)	0.0164 (5)	−0.0001 (5)	−0.0023 (4)	0.0004 (4)

Geometric parameters (Å, º)

Cl1—C11	1.7446 (14)	C6—H6A	0.9300
O1—C1	1.3543 (18)	C7—C8	1.4617 (18)
O1—C4	1.3691 (16)	C7—H7A	0.9300
O2—C5	1.2261 (18)	C8—C13	1.3974 (17)
C1—C2	1.356 (2)	C8—C9	1.410 (2)
C1—H1A	0.9300	C9—C10	1.384 (2)
C2—C3	1.422 (2)	C9—H9A	0.9300
C2—H2A	0.9300	C10—C11	1.388 (2)
C3—C4	1.370 (2)	C10—H10A	0.9300
C3—H3A	0.9300	C11—C12	1.386 (2)
C4—C5	1.4637 (18)	C12—C13	1.3865 (18)
C5—C6	1.4786 (18)	C12—H12A	0.9300
C6—C7	1.3388 (18)	C13—H13A	0.9300

C1—O1—C4	106.93 (11)	C6—C7—H7A	116.9
O1—C1—C2	111.03 (13)	C8—C7—H7A	116.9
O1—C1—H1A	124.5	C13—C8—C9	118.80 (12)
C2—C1—H1A	124.5	C13—C8—C7	119.30 (12)
C1—C2—C3	105.97 (14)	C9—C8—C7	121.90 (11)
C1—C2—H2A	127.0	C10—C9—C8	120.85 (12)
C3—C2—H2A	127.0	C10—C9—H9A	119.6
C4—C3—C2	106.68 (14)	C8—C9—H9A	119.6
C4—C3—H3A	126.7	C9—C10—C11	118.51 (12)
C2—C3—H3A	126.7	C9—C10—H10A	120.7
O1—C4—C3	109.39 (12)	C11—C10—H10A	120.7
O1—C4—C5	118.06 (12)	C12—C11—C10	122.24 (12)
C3—C4—C5	132.51 (13)	C12—C11—Cl1	119.52 (11)
O2—C5—C4	121.81 (12)	C10—C11—Cl1	118.23 (11)
O2—C5—C6	122.90 (13)	C11—C12—C13	118.71 (12)
C4—C5—C6	115.27 (12)	C11—C12—H12A	120.6
C7—C6—C5	121.11 (13)	C13—C12—H12A	120.6
C7—C6—H6A	119.4	C12—C13—C8	120.89 (12)
C5—C6—H6A	119.4	C12—C13—H13A	119.6
C6—C7—C8	126.29 (13)	C8—C13—H13A	119.6

C4—O1—C1—C2	0.69 (17)	C5—C6—C7—C8	−177.75 (13)
O1—C1—C2—C3	−0.41 (18)	C6—C7—C8—C13	−171.24 (14)
C1—C2—C3—C4	−0.02 (18)	C6—C7—C8—C9	9.4 (2)
C1—O1—C4—C3	−0.69 (16)	C13—C8—C9—C10	−0.2 (2)
C1—O1—C4—C5	177.19 (12)	C7—C8—C9—C10	179.11 (14)
C2—C3—C4—O1	0.44 (17)	C8—C9—C10—C11	0.2 (2)
C2—C3—C4—C5	−177.02 (15)	C9—C10—C11—C12	0.2 (2)
O1—C4—C5—O2	0.0 (2)	C9—C10—C11—Cl1	178.75 (11)
C3—C4—C5—O2	177.28 (16)	C10—C11—C12—C13	−0.6 (2)
O1—C4—C5—C6	−178.30 (12)	Cl1—C11—C12—C13	−179.09 (11)
C3—C4—C5—C6	−1.0 (2)	C11—C12—C13—C8	0.5 (2)
O2—C5—C6—C7	−6.2 (2)	C9—C8—C13—C12	−0.2 (2)
C4—C5—C6—C7	172.11 (14)	C7—C8—C13—C12	−179.49 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O2	0.93	2.52	2.8411 (17)	101
C13—H13*A*···O2^{i}	0.93	2.48	3.2535 (18)	140

Symmetry code: (i) −*x*, −*y*, *z*−1/2.