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Crystal structure of (*E*)-1-(3-chlorophenyl)-3-(furan-2-yl)prop-2-en-1-one

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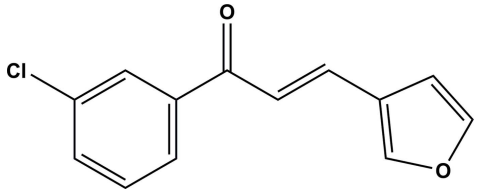
The title compound, $C_{13}H_9ClO_2$, exhibits a non-planar geometry; the furan ring being inclined to the benzene ring by 50.52 (16)°. In the crystal, molecules stack along the *a* axis; however, there are no significant intermolecular interactions present.

Keywords: crystal structure; chalcone.

CCDC reference: 1421581

1. Related literature

For the synthesis of the title compound, see: HanLee *et al.* (2011). For the syntheses of related compounds, see: Inokuma *et al.* (2009).



2. Experimental

2.1. Crystal data

$C_{13}H_9ClO_2$
M_r = 232.67
Monoclinic, $P2_1/c$
a = 7.186 (8) Å
b = 25.77 (3) Å
c = 5.774 (6) Å
β = 94.734 (10)°
V = 1066 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 173 K
0.30 × 0.30 × 0.10 mm

2.2. Data collection

Rigaku XtaLAB mini diffractometer
Absorption correction: multi-scan (REQAB; Rigaku, 1998)
T_{min} = 0.832, T_{max} = 0.967
11328 measured reflections
2461 independent reflections
1672 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.080

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.128
S = 1.07
2461 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *CrystalClear-SM Expert* (Rigaku, 2011); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2011); software used to prepare material for publication: *CrystalStructure*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5196).

References

HanLee, I.-S., Jeon, H.-J. & Lee, C.-K. (2011). *Bull. Korean Chem. Soc.* **32**, 687–692.
Rigaku (1998). *REQAB*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2011). *CrystalClear-SM Expert* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Inokuma, T., Nagamoto, Y., Sakamoto, S., Miyabe, H., Takasu, K. & Takemoto, Y. (2009). *Heterocycles*, **79**, 573–582.

supporting information

Acta Cryst. (2015). E**71**, o707 [doi:10.1107/S2056989015016266]

Crystal structure of (*E*)-1-(3-chlorophenyl)-3-(furan-2-yl)prop-2-en-1-one

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S1. Chemical context

The title compound is a chalcone analog that is currently being studied for its potential anticancer activity [unpublished results]. Its synthesis and NMR characteristics have been reported (HanLee *et al.* 2011), but its crystal structure has not been reported until now.

S2. Synthesis and crystallization

The title compound was synthesized by an aldol condensation reaction. 3-furaldehyde (1 mmol) and 3-chloroacetophenone (1 mmol) were dissolved in ethanol (5 ml). A NaOH solution (5 M, 1 mL) was added and the reaction mixture was stirred until a precipitate formed. The reaction mixture was cooled in an ice bath for 20 min. The solids formed were filtered off and recrystallized from MeOH/H_2O (1:1, v:v). Slow evaporation of a solution of the title compound in MeOH gave pale brown crystals.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The H atoms were included in calculated positions and treated as riding atoms: C—H = 0.95 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

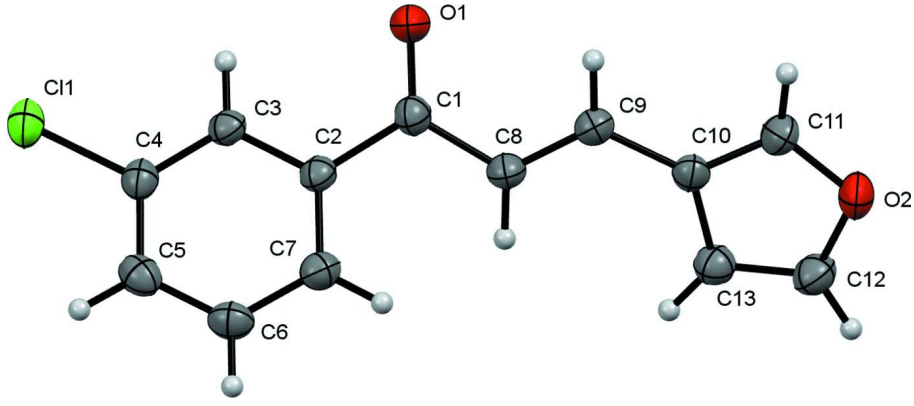

Figure 1

A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

(*E*)-1-(3-Chlorophenyl)-3-(furan-2-yl)prop-2-en-1-one

Crystal data

$C_{13}H_9ClO_2$
$M_r = 232.67$

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 7.186 (8) Å
b = 25.77 (3) Å
c = 5.774 (6) Å
β = 94.734 (10)°
V = 1066 (2) Å^3
Z = 4
F(000) = 480.00
D_x = 1.450 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 2235 reflections
θ = 2.4–27.5°
μ = 0.34 mm^{-1}
T = 173 K
Prism, colorless
0.30 × 0.30 × 0.10 mm

Data collection

Rigaku XtaLAB mini diffractometer
Detector resolution: 6.827 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (REQAB; Rigaku, 1998)
T_{min} = 0.832, T_{max} = 0.967
11328 measured reflections

2461 independent reflections
1672 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.080
θ_{max} = 27.6°
h = −9→9
k = −33→33
l = −7→7

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.128
S = 1.07
2461 reflections
145 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.6811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.25413 (11)	0.29816 (3)	0.35320 (13)	0.0404 (3)
O1	0.2759 (3)	0.50459 (7)	0.3133 (4)	0.0385 (6)
O2	0.3111 (3)	0.71261 (7)	0.9248 (4)	0.0395 (5)
C1	0.2650 (4)	0.49620 (10)	0.5220 (5)	0.0295 (6)
C2	0.2198 (4)	0.44238 (10)	0.6022 (5)	0.0263 (6)
C3	0.2537 (4)	0.40038 (10)	0.4594 (5)	0.0271 (6)
C4	0.2074 (4)	0.35117 (10)	0.5274 (5)	0.0289 (6)
C5	0.1236 (4)	0.34244 (11)	0.7323 (5)	0.0335 (7)
C6	0.0897 (4)	0.38439 (11)	0.8733 (5)	0.0334 (7)
C7	0.1396 (4)	0.43435 (11)	0.8108 (5)	0.0304 (7)
C8	0.2914 (4)	0.53727 (10)	0.6976 (5)	0.0293 (6)
C9	0.2727 (4)	0.58734 (10)	0.6361 (5)	0.0271 (6)
C10	0.3055 (4)	0.63097 (10)	0.7933 (5)	0.0275 (6)
C11	0.2624 (4)	0.68115 (11)	0.7414 (5)	0.0338 (7)

C12	0.3882 (5)	0.68125 (12)	1.0974 (5)	0.0369 (7)
C13	0.3873 (4)	0.63144 (11)	1.0275 (5)	0.0327 (7)
H3	0.3082	0.4057	0.3168	0.0325*
H5	0.0902	0.3083	0.7751	0.0402*
H6	0.0320	0.3790	1.0135	0.0400*
H7	0.1190	0.4628	0.9100	0.0365*
H8	0.3220	0.5284	0.8559	0.0352*
H9	0.2353	0.5948	0.4780	0.0325*
H11	0.2058	0.6927	0.5960	0.0406*
H12	0.4359	0.6930	1.2466	0.0443*
H13	0.4323	0.6023	1.1162	0.0393*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0503 (5)	0.0258 (4)	0.0454 (5)	0.0004 (4)	0.0067 (4)	−0.0059 (3)
O1	0.0601 (15)	0.0292 (11)	0.0266 (11)	0.0010 (10)	0.0055 (10)	0.0005 (9)
O2	0.0520 (13)	0.0243 (11)	0.0418 (12)	−0.0012 (10)	0.0011 (10)	−0.0057 (9)
C1	0.0321 (15)	0.0254 (14)	0.0308 (15)	0.0027 (12)	0.0017 (12)	−0.0006 (12)
C2	0.0285 (14)	0.0268 (14)	0.0231 (13)	0.0008 (12)	−0.0017 (11)	−0.0017 (11)
C3	0.0289 (15)	0.0297 (15)	0.0224 (14)	−0.0024 (12)	0.0002 (11)	−0.0026 (11)
C4	0.0294 (15)	0.0258 (14)	0.0308 (15)	0.0019 (12)	−0.0023 (12)	−0.0024 (12)
C5	0.0319 (16)	0.0331 (16)	0.0347 (16)	−0.0032 (13)	−0.0026 (13)	0.0051 (12)
C6	0.0314 (16)	0.0391 (17)	0.0302 (15)	−0.0022 (13)	0.0065 (12)	0.0035 (13)
C7	0.0311 (15)	0.0339 (16)	0.0262 (14)	0.0024 (13)	0.0023 (12)	−0.0014 (12)
C8	0.0351 (16)	0.0285 (14)	0.0239 (14)	0.0001 (13)	−0.0001 (11)	0.0000 (11)
C9	0.0272 (14)	0.0294 (14)	0.0247 (14)	0.0002 (12)	0.0022 (11)	−0.0014 (11)
C10	0.0287 (14)	0.0271 (14)	0.0275 (14)	−0.0018 (12)	0.0062 (11)	−0.0008 (11)
C11	0.0397 (17)	0.0307 (15)	0.0304 (15)	−0.0047 (13)	−0.0009 (13)	−0.0035 (12)
C12	0.0419 (18)	0.0388 (17)	0.0295 (15)	0.0016 (15)	−0.0007 (13)	−0.0049 (13)
C13	0.0338 (16)	0.0335 (16)	0.0307 (15)	0.0020 (14)	0.0008 (12)	0.0002 (12)

Geometric parameters (Å, º)

Cl1—C4	1.746 (3)	C4—C5	1.389 (5)
O1—C1	1.233 (4)	C5—C6	1.387 (5)
O2—C11	1.357 (4)	C6—C7	1.392 (5)
O2—C12	1.365 (4)	C8—C9	1.342 (4)
C1—C2	1.506 (4)	C9—C10	1.452 (4)
C1—C8	1.467 (4)	C10—C11	1.357 (4)
C2—C3	1.394 (4)	C10—C13	1.429 (4)
C2—C7	1.393 (4)	C12—C13	1.346 (5)
C3—C4	1.377 (4)		
C11—O2—C12	106.2 (3)	C4—C5—C6	118.9 (3)
O1—C1—C2	119.7 (3)	C5—C6—C7	120.5 (3)
O1—C1—C8	122.3 (3)	C2—C7—C6	119.7 (3)
C2—C1—C8	118.1 (3)	C1—C8—C9	120.4 (3)

C1—C2—C3	118.7 (3)	C8—C9—C10	124.9 (3)
C1—C2—C7	121.2 (3)	C9—C10—C11	125.3 (3)
C3—C2—C7	120.1 (3)	C9—C10—C13	129.1 (3)
C2—C3—C4	119.2 (3)	C11—C10—C13	105.6 (3)
Cl1—C4—C3	119.6 (3)	O2—C11—C10	110.9 (3)
Cl1—C4—C5	118.8 (3)	O2—C12—C13	110.7 (3)
C3—C4—C5	121.6 (3)	C10—C13—C12	106.5 (3)