Crystal structure of the chalcone (*E*)-3-(furan-2-yl)-1-phenylprop-2-en-1-one

Oscar F. Vázquez-Vuelvas,[a]‡ René A. Enríquez-Figueroa,[a] Héctor García-Ortega,[b] Marcos Flores-Alamo[b] and Armando Pineda-Contreras[a]*

[a]Facultad de Ciencias Químicas, Universidad de Colima, Km 9 Carr. Colima-Coquimatlán s/n, Coquimatlán, Colima 28400, Mexico, and [b]Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, México, DF 04510, Mexico. *Correspondence e-mail: armandop@ucol.mx

The title chalcone derivative, $C_{13}H_{10}O_2$, adopts an *E* conformation about the C=C double bond. The molecule is composed of a furanyl and a phenyl ring, bridged by an α,β-unsaturated carbonyl system, which are inclined to one another by 24.07 (7)°. In the crystal, molecules are connected by weak C—H···O hydrogen bonds involving the carbonyl O atom acting as a trifurcated acceptor and C—H···π interactions, forming ribbons extending along the *c*-axis direction.

1. Chemical context

The Claisen–Schmidt condensation reaction between substituted acetophenones and aryl aldehydes under basic conditions has been widely used to synthesize chalcone derivatives (Ghosh & Das, 2014; Robinson *et al.*, 2013; Sharma *et al.*, 2013; Tiwari *et al.*, 2010). Chalcones, belonging to the flavonoid family, are an important class of natural products with widespread distribution in fruits, vegetables, spices and tea. These compounds are also often used as the precursors for the synthesis of various heterocyclic compounds (Chimenti *et al.*, 2010; Elarfi & Al-Difar, 2012; Ghosh & Das, 2014; Hamada & Sharshira, 2011; Mahé *et al.*, 2012; Sharma *et al.*, 2013). Chemically, chalcones are 1,3-diaryl-2-propen-1-ones in which two aromatic rings, mainly benzene groups, are joined by a three-carbon bridge having a carbonyl moiety and α,β-unsaturation.

Many studies have shown that chalcone derivatives exhibit a wide range of pharmacological activities, such as potential cytotoxic, antimicrobial, antiviral, anti-inflammatory, antioxidant, anaesthetic, antimalarial, antileishmanial, antitubercular, antitumor and anticancer activities (Boeck *et al.*, 2006; Chimenti *et al.*, 2010; Elarfi & Al-Difar, 2012; Hamada & Sharshira, 2011; Hsieh *et al.*, 2000; Kumar *et al.*, 2003; Sharma *et al.*, 2013). These versatile compounds and their furan derivatives are often used as intermediates in the syntheses of monoamine oxidase (MAO) inhibitors; moreover, the chalcones themselves have MAO inhibitory activity. Since the furan moiety represents a high π-electron density that contributes to the interaction with the flavin nucleus of the cofactor in the inhibition of MAO, some furan-substituted chalcones, where an electron-rich heterocyclic oxygen replaces the benzene ring, have been synthesized to investigate their biological activity (Robinson *et al.*, 2013; Shaikh *et al.*, 2014; Sharma *et al.*, 2013; Zheng *et al.*, 2011). In view of the varied biological and pharmacological applications, we report
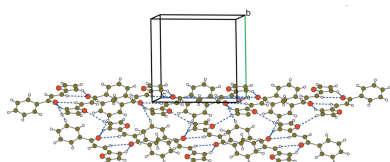
herein on the synthesis and the molecular and supramolecular structure of the title compound, synthesized by a conventional base-catalysed Claisen–Schmidt condensation reaction.
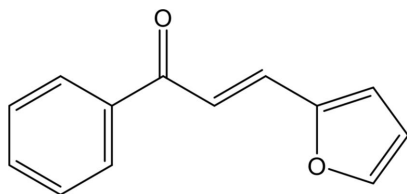
2. Structural commentary

The symmetry-independent molecule adopts an *E* conformation corresponding to an α,β-unsaturated non-planar structure, which bridges the pair of aromatic groups (Fig. 1). The two main planar groups, the furanyl and the phenyl rings, form a dihedral angle of 24.07 (7)°. In this context, the molecular structure can be considered, for descriptive purposes, as two fragments basically described by the furanyl acryloyl and the benzoyl moieties. The benzoyl group shows a non-planar structure and presents rotation when observing the C2—C1—C7—O2 torsion angle of 19.4 (2)°, denoting a marked deviation from planarity at the C1—C7 bond, a single bond with rotational freedom. This deviation from planarity has also been reported previously in the crystal structure of an (*E*)-3-(4-hydroxyphenyl)-1-(4-methoxyphenyl)-prop-2-en-1-one derivative, when observing the analogous reported interplanar angle shown in the respectively 4-methoxybenzoyl moiety (Qiu *et al.*, 2006). In the same manner, the furanyl acryloyl entity presents a quasi-planar structure indicated by the two small torsion angles O2—C7—C8—C9 [−5.4 (2)°] and C7—C8—C9—C10 [−176.31 (13)°], similar to the structure of the difuranyl chalcone derivative (*E*)-1,3-di(2-furyl)-2-propen-1-one (Ocak Iskeleli *et al.*, 2005*b*). On the other hand, the molecule interatomic linkage coincides with similar reported structures, specifically in the α,β-unsaturated entity of the title crystal (Harrison *et al.*, 2006; Ocak Iskeleli *et al.*, 2005*a,b*). As a result, the interatomic distances are in agreement with the conjugative nature, which is additionally supported by other
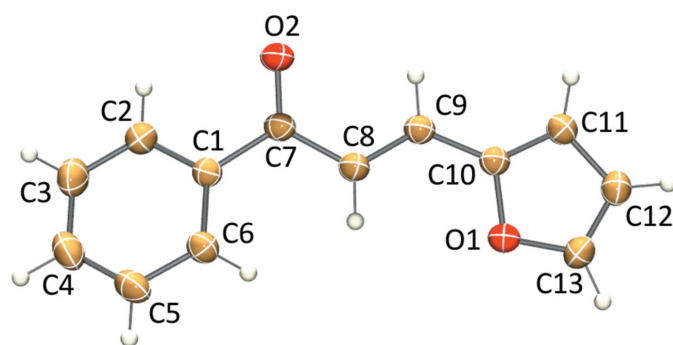
Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the O1/C10–C13 furanyl ring and the C1–C6 phenyl ring, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots$O2[i]	0.95	2.51	3.457 (2)	151
C9—H9$\cdots$O2[ii]	0.95	2.62	3.416 (1)	142
C11—H11$\cdots$O2[ii]	0.95	2.51	3.277 (2)	138
C6—H6$\cdots$Cg1[iii]	0.95	2.88	3.687 (2)	144
C13—H13$\cdots$Cg2[iv]	0.95	2.71	3.519 (9)	143

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

described types of different weak interactions (*vide infra*) and also define the characteristic quasi-planar structure of chalcone derivatives.

3. Supramolecular features

The crystal packing does not present geometrical parameters corresponding to classical hydrogen bonding (Gilli & Gilli, 2009; Steiner, 2002), neither intra- nor intermolecular. In the crystal, centrosymmetrically related molecules interact through a pair of weak hydrogen contacts (Table 1) with the C9 and C11 carbon atoms as donors and the O2 oxygen atom as a bifurcated acceptor, generating a ring with an $R_2^1(6)$ graph-set motif (Bernstein *et al.*, 1995). The reciprocal interactions with the corresponding molecule positioned in a head-to-tail mode generate the same ring motif and, as a consequence, an $R_2^2(10)$ ring is formed, describing a three-fused-ring system (Fig. 2). In addition, a weak hydrogen contact is present involving the C3 carbon atom as H-donor and the O2 oxygen atom acting, in this way, as a trifurcated acceptor. The propagation of this interaction generates a ribbon along the *c*-axis direction (Fig. 2). The supramolecular assembly is additionally supported by weak C—H$\cdots\pi$ interactions, implicating the phenyl and furanyl π systems (Fig. 3).

4. Synthesis and crystallization

To a solution of NaOH (2.18 g, 55 mmol) in H$_2$O/EtOH (30 ml, 2:1 *v/v*) was added pure acetophenone (5.2 g,

Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.
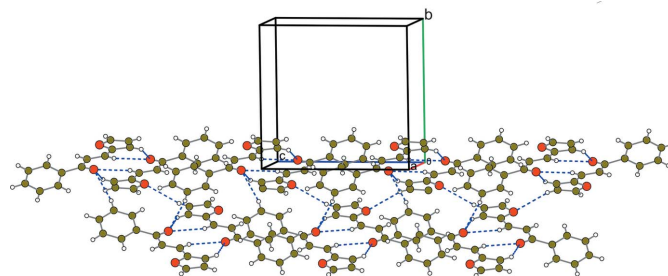

Figure 2
A partial packing diagram of the title compound, showing the hydrogen-bonded supramolecular assembly *via* C—H$\cdots$O interactions (blue dashed lines).
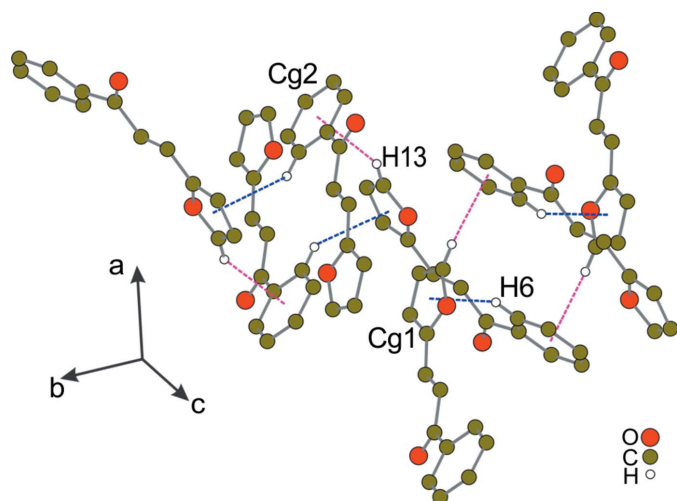
Crystal data	
Chemical formula	$C_{13}H_{10}O_2$
M_r	198.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	130
a, b, c (Å)	9.5296 (7), 10.1383 (7), 11.1595 (7)
β (°)	103.922 (6)
V (Å^3)	1046.49 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	$0.50 \times 0.45 \times 0.32$
Data collection	
Diffractometer	Agilent Xcalibur Atlas Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min}, T_{max}	0.781, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8114, 2553, 1755
R_{int}	0.019
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.691
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.115, 1.04
No. of reflections	2553
No. of parameters	136
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.11, −0.17

Computer programs: *CrysAlis PRO* (Agilent, 2011), *SHELXS2013* and *SHELXL2013* (Sheldrick, 2008, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2006) and *DIAMOND* (Brandenburg, 2012).

Figure 3
A partial packing diagram of the title compound, showing the C—H···π stacking interactions, depicted as blue and purple dotted lines for the C6—H6···*Cg*1 and C13—H13···*Cg*2 contacts, respectively. H atoms not involved in hydrogen-bonding interactions have been omitted for clarity.

43 mmol), and stirring started; furfuraldehyde (4.6 g, 43 mmol) was then added at once. The reaction mixture was stirred for two hours and then kept in a refrigerator overnight. The resulting product was separated and then distilled under vacuum. The title compound was obtained as a yellow solid in 82% yield. Single-crystals suitable for X-ray determination were obtained by evaporation of an ethyl ether solution. M.p. 311–313 K; IR (ν, cm^{-1}): 3123 (C—H$_{alk}$), 3035 (C—H$_{arom}$), 1658 (C=O), 1594, 1545, 1474 (C=C). ^{1}H NMR (400 MHz, CDCl$_3$, δ, p.p.m.): 8.04 (2H, *dd*), 7.61 (1H, *d*), 7.58 (1H, *tt*), 7.52 (2H, *dd*), 7.49 (1H, *dd*), 7.47 (1H, *d*), 6.72 (1H, *dd*), 6.51 (1H, *dd*). ^{13}C NMR (100 MHz, CDCl$_3$, δ, p.p.m.): 189.85 (C7), 151.69 (C10), 144.98 (C13), 138.16 (C1), 132.82 (C4), 130.72 (C9), 128.65 (C2,6), 128.47 (C3,5), 119.30 (C8), 116.33 (C11), 112.74 (C12). MS m/z: 199 (M +1); Analysis calculated for $C_{13}H_{10}O_2$: C, 78.78; H, 5.05. Found: 78.80; H, 5.09.

5. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C atoms were placed in geometrically idealized positions and refined as riding on their parent atoms, with C—H = 0.95 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Acknowledgements

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Boeck, P., Bandeira Falcão, C. A., Leal, P. C., Yunes, R. A., Filho, V. C., Torres-Santos, E. C. & Rossi-Bergmann, B. (2006). *Bioorg. Med. Chem.* **14**, 1538–1545.
Brandenburg, K. (2012). *DIAMOND*. Crystal Impact GbR. Bonn, Germany.
Chimenti, F., Fioravanti, R., Bolasco, A., Chimenti, P., Secci, D., Rossi, F., Yáñez, M., Orallo, F., Ortuso, F., Alcaro, S., Cirilli, R., Ferretti, R. & Sanna, M. L. (2010). *Bioorg. Med. Chem.* **18**, 1273–1279.
Elarfi, M. J. & Al-Difar, H. A. (2012). *Sci. Rev. Chem. Commun.* **2**, 103–107.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Ghosh, R. & Das, A. (2014). *World J. Pharm. Pharma. Sci.* **3**, 578–595.
Gilli, G. & Gilli, P. (2009). *The Nature of the Hydrogen Bond: Outline of a Comprehensive Hydrogen Bond Theory*. Oxford: International Union of Crystallography and Oxford Science Publications.
Hamada, N. M. & Sharshira, E. M. (2011). *Molecules*, **16**, 2304–2312.
Harrison, W. T. A., Yathirajan, H. S., Anilkumar, H. G., Sarojini, B. K. & Narayana, B. (2006). *Acta Cryst.* E**62**, o3251–o3253.
Hsieh, H.-K., Tsao, L.-T., Wang, J. P. & Lin, C. N. (2000). *J. Pharm. Pharmacol.* **52**, 163–171.
Kumar, S. K., Hager, E., Pettit, C., Gurulingappa, H., Davidson, N. E. & Khan, S. R. (2003). *J. Med. Chem.* **46**, 2813–2815.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Mahé, O., Dez, I., Levacher, V. & Brière, J. F. (2012). *Org. Biomol. Chem.* **10**, 3946–3954.
Ocak İskeleli, N., Işık, Ş., Özdemir, Z. & Bilgin, A. (2005a). *Acta Cryst.* E**61**, o1278–o1279.
Ocak İskeleli, N., Işık, S., Özdemir, Z. & Bilgin, A. (2005b). *Acta Cryst.* E**61**, o1356–o1358.
Qiu, X.-Y., Yang, S.-L., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o3324–o3325.

research communications

Robinson, S. J., Petzer, J. P., Petzer, A., Bergh, J. J. & Lourens, A. C. U. (2013). *Bioorg. Med. Chem. Lett.* **23**, 4985–4989.

Shaikh, S. B., Mujahid, S., Tambat, N., Salgar, K. & Nimbale, R. V. (2014). *Int. J. Pharm. Res. Sch.* **3**, 317–329.

Sharma, P., Kumar, S., Ali, F., Anthal, S., Gupta, V., Khan, I., Singh, S., Sangwan, P., Suri, K., Gupta, B., Gupta, D., Dutt, P., Vishwakarma, R. & Satti, N. (2013). *Med. Chem. Res.* **22**, 3969–3983.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Steiner, T. (2002). *Angew. Chem. Int. Ed.* **41**, 48–76.

Tiwari, B., Pratapwar, A. S., Tapas, A. R. & Butle, S. R. (2010). *Int. J. ChemTech Res.* **2**, 499–503.

Zheng, C. J., Jiang, S.-M., Chen, Z. H., Ye, B.-J. & Piao, H. R. (2011). *Arch. Pharm. Pharm. Med. Chem.* **344**, 689–695.

supporting information

Crystal structure of the chalcone (*E*)-3-(furan-2-yl)-1-phenylprop-2-en-1-one

Oscar F. Vázquez-Vuelvas, René A. Enríquez-Figueroa, Héctor García-Ortega, Marcos Flores-Alamo and Armando Pineda-Contreras

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008, 2015); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *DIAMOND* (Brandenburg, 2012) and *WinGX* (Farrugia, 2012).

(*E*)-3-(Furan-2-yl)-1-phenylprop-2-en-1-one

Crystal data

$C_{13}H_{10}O_2$	$F(000) = 416$
$M_r = 198.21$	$D_x = 1.258$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2252 reflections
$a = 9.5296$ (7) Å	$\theta = 3.8–29.4°$
$b = 10.1383$ (7) Å	$\mu = 0.08$ mm^{-1}
$c = 11.1595$ (7) Å	$T = 130$ K
$\beta = 103.922$ (6)°	Prism, colorless
$V = 1046.49$ (13) Å^3	$0.50 \times 0.45 \times 0.32$ mm
$Z = 4$	

Data collection

Agilent Xcalibur Atlas Gemini diffractometer	8114 measured reflections
	2553 independent reflections
Graphite monochromator	1755 reflections with $I > 2\sigma(I)$
Detector resolution: 10.4685 pixels mm^{-1}	$R_{int} = 0.019$
ω scans	$\theta_{max} = 29.4°$, $\theta_{min} = 3.8°$
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)	$h = -12 \rightarrow 11$
	$k = -13 \rightarrow 14$
$T_{min} = 0.781$, $T_{max} = 1$	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.1328P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
2553 reflections	$(\Delta/\sigma)_{max} < 0.001$
136 parameters	$\Delta\rho_{max} = 0.11$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlisPro, Agilent Technologies (Agilent, 2011) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.96039 (10)	0.15914 (10)	0.09922 (8)	0.0619 (3)
C1	0.65936 (13)	−0.05129 (13)	0.39220 (11)	0.0465 (3)
O2	0.50969 (10)	−0.03589 (12)	0.19207 (8)	0.0724 (3)
C7	0.62831 (14)	−0.01269 (13)	0.25976 (11)	0.0499 (3)
C9	0.72460 (14)	0.06998 (13)	0.09060 (12)	0.0498 (3)
H9	0.6322	0.049	0.0396	0.06*
C8	0.74268 (14)	0.04814 (14)	0.21095 (11)	0.0516 (3)
H8	0.8312	0.0724	0.2662	0.062*
C10	0.82803 (14)	0.12119 (13)	0.02963 (11)	0.0477 (3)
C11	0.82469 (15)	0.13668 (14)	−0.09089 (12)	0.0549 (3)
H11	0.7452	0.1182	−0.1585	0.066*
C6	0.76975 (15)	0.00494 (14)	0.48148 (12)	0.0551 (4)
H6	0.8309	0.0694	0.4587	0.066*
C12	0.96066 (16)	0.18535 (14)	−0.09817 (13)	0.0587 (4)
H12	0.991	0.2057	−0.1711	0.07*
C2	0.57275 (16)	−0.14617 (15)	0.42759 (13)	0.0605 (4)
H2	0.4966	−0.1857	0.3675	0.073*
C13	1.03802 (17)	0.19718 (16)	0.01731 (14)	0.0649 (4)
H13	1.1349	0.2281	0.0399	0.078*
C5	0.79115 (17)	−0.03262 (17)	0.60379 (13)	0.0674 (4)
H5	0.8662	0.0069	0.6649	0.081*
C4	0.70484 (19)	−0.12620 (19)	0.63691 (15)	0.0745 (5)
H4	0.72	−0.1517	0.721	0.089*
C3	0.59661 (19)	−0.18335 (18)	0.54951 (16)	0.0740 (5)
H3	0.5375	−0.2492	0.573	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0544 (6)	0.0759 (7)	0.0512 (5)	−0.0135 (5)	0.0044 (4)	0.0031 (5)
C1	0.0452 (7)	0.0491 (7)	0.0454 (7)	0.0025 (5)	0.0115 (5)	−0.0024 (5)
O2	0.0504 (6)	0.1151 (9)	0.0482 (6)	−0.0173 (6)	0.0049 (4)	−0.0038 (6)
C7	0.0457 (7)	0.0577 (8)	0.0448 (7)	−0.0021 (6)	0.0080 (5)	−0.0071 (6)
C9	0.0469 (7)	0.0538 (8)	0.0471 (7)	−0.0012 (6)	0.0085 (5)	−0.0031 (6)
C8	0.0476 (7)	0.0602 (8)	0.0455 (7)	−0.0060 (6)	0.0081 (5)	−0.0030 (6)
C10	0.0470 (7)	0.0475 (7)	0.0468 (7)	−0.0015 (5)	0.0078 (5)	−0.0010 (5)
C11	0.0556 (8)	0.0610 (8)	0.0473 (7)	−0.0025 (7)	0.0110 (6)	−0.0014 (6)

C6	0.0585 (8)	0.0595 (8)	0.0467 (7)	−0.0017 (6)	0.0113 (6)	−0.0054 (6)
C12	0.0610 (9)	0.0609 (9)	0.0582 (8)	0.0001 (7)	0.0217 (7)	0.0050 (7)
C2	0.0546 (8)	0.0661 (9)	0.0605 (9)	−0.0038 (7)	0.0129 (6)	0.0034 (7)
C13	0.0533 (8)	0.0721 (10)	0.0702 (10)	−0.0104 (7)	0.0164 (7)	0.0086 (8)
C5	0.0675 (10)	0.0847 (11)	0.0461 (8)	0.0074 (8)	0.0060 (7)	−0.0061 (8)
C4	0.0788 (11)	0.0943 (13)	0.0523 (9)	0.0182 (10)	0.0193 (8)	0.0168 (9)
C3	0.0742 (11)	0.0777 (11)	0.0742 (11)	0.0007 (8)	0.0256 (9)	0.0199 (9)

Geometric parameters (Å, º)

O1—C13	1.3627 (17)	C11—H11	0.95
O1—C10	1.3678 (15)	C6—C5	1.3840 (19)
C1—C2	1.3855 (19)	C6—H6	0.95
C1—C6	1.3857 (18)	C12—C13	1.327 (2)
C1—C7	1.4882 (17)	C12—H12	0.95
O2—C7	1.2218 (15)	C2—C3	1.377 (2)
C7—C8	1.4664 (18)	C2—H2	0.95
C9—C8	1.3308 (17)	C13—H13	0.95
C9—C10	1.4236 (18)	C5—C4	1.364 (2)
C9—H9	0.95	C5—H5	0.95
C8—H8	0.95	C4—C3	1.366 (2)
C10—C11	1.3468 (18)	C4—H4	0.95
C11—C12	1.407 (2)	C3—H3	0.95
C13—O1—C10	105.91 (10)	C5—C6—H6	119.9
C2—C1—C6	118.81 (12)	C1—C6—H6	119.9
C2—C1—C7	118.43 (11)	C13—C12—C11	106.25 (13)
C6—C1—C7	122.76 (12)	C13—C12—H12	126.9
O2—C7—C8	120.74 (12)	C11—C12—H12	126.9
O2—C7—C1	119.78 (12)	C3—C2—C1	120.25 (14)
C8—C7—C1	119.44 (11)	C3—C2—H2	119.9
C8—C9—C10	127.34 (12)	C1—C2—H2	119.9
C8—C9—H9	116.3	C12—C13—O1	111.18 (13)
C10—C9—H9	116.3	C12—C13—H13	124.4
C9—C8—C7	121.16 (12)	O1—C13—H13	124.4
C9—C8—H8	119.4	C4—C5—C6	120.22 (15)
C7—C8—H8	119.4	C4—C5—H5	119.9
C11—C10—O1	109.34 (12)	C6—C5—H5	119.9
C11—C10—C9	131.84 (12)	C5—C4—C3	120.17 (14)
O1—C10—C9	118.76 (11)	C5—C4—H4	119.9
C10—C11—C12	107.32 (12)	C3—C4—H4	119.9
C10—C11—H11	126.3	C4—C3—C2	120.40 (16)
C12—C11—H11	126.3	C4—C3—H3	119.8
C5—C6—C1	120.15 (14)	C2—C3—H3	119.8
C2—C1—C7—O2	19.4 (2)	C9—C10—C11—C12	−176.65 (14)
C6—C1—C7—O2	−159.66 (14)	C2—C1—C6—C5	−0.7 (2)
C2—C1—C7—C8	−158.15 (13)	C7—C1—C6—C5	178.37 (13)

C6—C1—C7—C8	22.74 (19)	C10—C11—C12—C13	−0.29 (17)
C10—C9—C8—C7	−176.31 (13)	C6—C1—C2—C3	0.0 (2)
O2—C7—C8—C9	−5.4 (2)	C7—C1—C2—C3	−179.11 (14)
C1—C7—C8—C9	172.14 (12)	C11—C12—C13—O1	−0.03 (18)
C13—O1—C10—C11	−0.50 (16)	C10—O1—C13—C12	0.33 (17)
C13—O1—C10—C9	177.07 (12)	C1—C6—C5—C4	0.8 (2)
C8—C9—C10—C11	173.72 (14)	C6—C5—C4—C3	−0.1 (2)
C8—C9—C10—O1	−3.2 (2)	C5—C4—C3—C2	−0.7 (3)
O1—C10—C11—C12	0.49 (16)	C1—C2—C3—C4	0.7 (3)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the O1/C10–C13 furanyl ring and the C1–C6 phenyl ring, respectively.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3⋯O2[i]	0.95	2.51	3.457 (2)	151
C9—H9⋯O2[ii]	0.95	2.62	3.416 (1)	142
C11—H11⋯O2[ii]	0.95	2.51	3.277 (2)	138
C6—H6⋯Cg1[iii]	0.95	2.88	3.687 (2)	144
C13—H13⋯Cg2[iv]	0.95	2.71	3.519 (9)	143

Symmetry codes: (i) x, $-y-1/2$, $z+1/2$; (ii) $-x+1$, $-y$, $-z$; (iii) x, $-y+1/2$, $z+1/2$; (iv) $-x-2$, $y+1/2$, $-z+1/2$.