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Steric repulsion and supramolecular assemblies *via* a two-dimensional plate by C—H⋯O hydrogen bonds in two closely related 2-(benzofuran-2-yl)-2-oxoethyl benzoates

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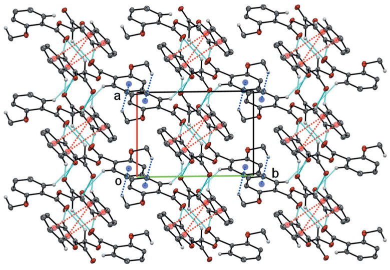
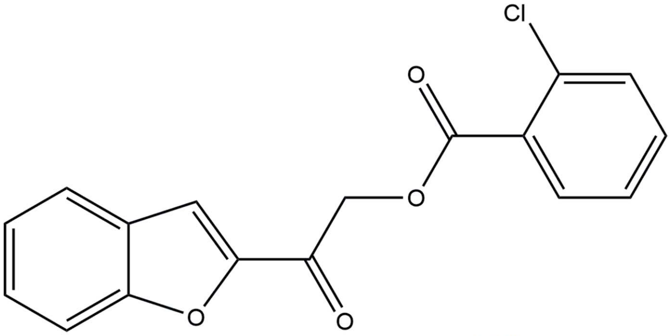
2-(Benzofuran-2-yl)-2-oxoethyl 2-chlorobenzoate, $C_{17}H_{11}ClO_4$ (I), and 2-(benzofuran-2-yl)-2-oxoethyl 2-methoxybenzoate, $C_{18}H_{14}O_5$ (II), were synthesized under mild conditions. Their chemical and molecular structures were analyzed by spectroscopic and single-crystal X-ray diffraction studies, respectively. These compounds possess different *ortho*-substituted functional groups on their phenyl rings, thus experiencing extra steric repulsion force within their molecules as the substituent changes from 2-chloro (I) to 2-methoxy (II). The crystal packing of compound (I) depends on weak intermolecular hydrogen bonds and π–π interactions. Molecules are related by inversion into centrosymmetric dimers *via* C—H⋯O hydrogen bonds, and further strengthened by π–π interactions between furan rings. Conversely, molecules in compound (II) are linked into alternating dimeric chains propagating along the [101] direction, which develop into a two-dimensional plate through extensive intermolecular hydrogen bonds. These plates are further stabilized by π–π and C—H⋯π interactions.

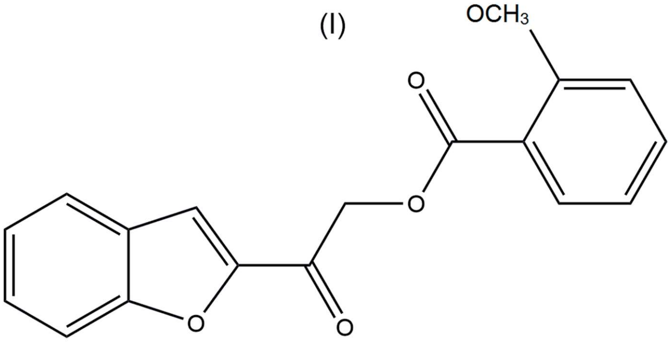


1. Chemical context

Benzofurans are an important class of heterocyclic compounds with fused benzene and furan rings. The benzofuran nucleus has been widely used as the building block for various biologically active compounds due to its broad range of pharmacological properties (Swamy *et al.*, 2015; Zhou *et al.*, 2010; Rangaswamy *et al.*, 2012). Benzofuran derivatives, especially with substituents at their C-2 position, are commonly found in natural products and synthetic compounds. Several reviews describing the biological potential of these scaffolds acting as antioxidant (Chand *et al.*, 2017), antimicrobial (Hiremathad *et al.*, 2015), anticancer and antiviral (Khanam & Shamsuzzaman, 2015) agents have been published. Encouraged by previous studies, we are herein reporting the synthesis, spectroscopic studies and structure determination of 2-(benzofuran-2-yl)-2-oxoethyl 2-chlorobenzoate (I) and 2-(benzofuran-2-yl)-2-oxoethyl 2-methoxybenzoate (II).



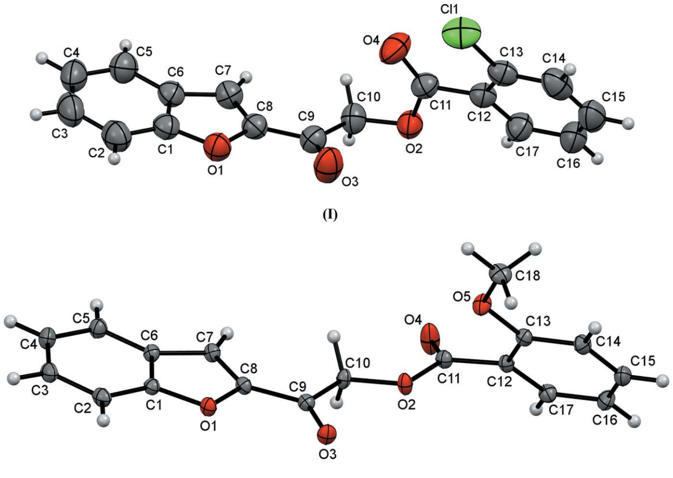
(I)



(II)

2. Structural commentary

The molecular structure of the title compounds (Fig. 1) contain two ring systems, which are the benzofuran and the *ortho*-substituted [chloro- for (I) and methoxy- for (II)] phenyl rings, interconnected by a C—C(=O)—O—C(=O) connecting bridge. The unique molecular conformations of compounds (I) and (II) can be characterized by three torsion angles, *i.e.* $\tau1$ (O1—C8—C9—O3), $\tau2$ (C9—C10—O2—C11) and $\tau3$ (O4—C11—C12—C13) respectively (Fig. 2). The torsion angle $\tau1$ for both structures is approximately 0°, signifying the coplanarity between their benzofuran ring and the adjacent carbonyl group at the connecting bridge. As for the torsion angle between the two carbonyl groups, $\tau2$, compound (I) exhibits a *syn-clinal* conformation [C9—C10—O2—C11 = −76.19 (17)°] whereas compound (II) adopts an *anti-periplanar* conformation [C9—C10—O2—C11 = −173.51 (9)°]. Likewise, owing to the *ortho*-substitution of the functional group at their phenyl rings, both studied compounds experience steric repulsion between their substituent and adjacent carbonyl groups, which can influence torsion angle $\tau3$. Greater steric repulsion force is observed between carbonyl group and methoxy groups [O4—C11—C12—C13 = 123.09 (14)° for compound (II)] than with the chlorine atom [O4—C11—C12—C13 = 22.0 (3)° for compound (I)] (Then *et al.*, 2017).



(I)

(II)

Figure 1
The structures of (I) and (II), showing 50% probability displacement ellipsoids and the atomic labelling scheme.

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O4^{i}	0.97	2.53	3.495 (2)	176

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

$Cg3$ is the centroid of the C12–C17 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O3^{i}	0.95	2.45	3.2677 (15)	145
C7—H7A···O4^{ii}	0.95	2.31	3.2352 (16)	163
C10—H10A···O3^{iii}	0.99	2.55	3.3746 (14)	141
C10—H10B···O4^{ii}	0.99	2.44	3.2028 (17)	134
C17—H17A···O1^{iii}	0.95	2.55	3.2730 (15)	134
C18—H18C···$Cg3^{iv}$	0.98	2.81	3.6181 (16)	141

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

3. Supramolecular features

The crystal packing of compound (I) features weak intermolecular hydrogen bonds (Table 1) and π–π interactions. Two inversion-related molecules are joined to form a centrosymmetric dimer by a pair of weak intermolecular C10—H10B···O4 hydrogen bonds, generating an $R_2^2(10)$ graph-set motif (Fig. 3). These dimers are further consolidated by π–π

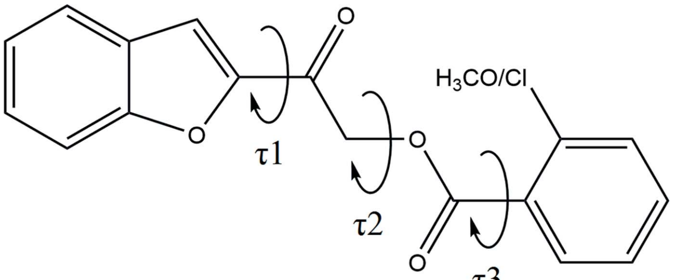


Figure 2
General chemical diagram showing the torsion angles $\tau1$, $\tau2$ and $\tau3$.

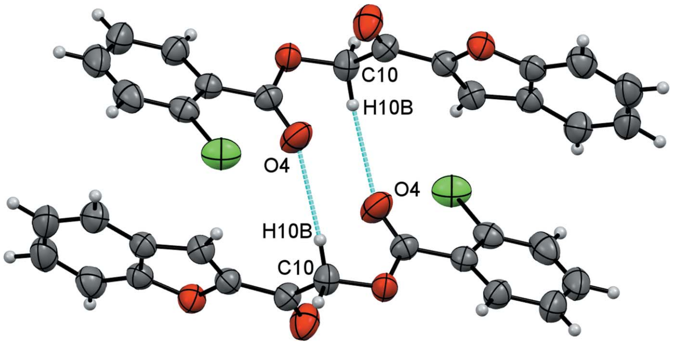


Figure 3
The dimeric structure of compound (I) formed by two adjacent inversion-related molecules.

interactions, involving two face-to-face related furan rings, distanced by 3.6623 (11) Å, propagating along the [001] direction (Fig. 4) with symmetry code $-x + 1$, $-y + 1$, $-z + 1$.

Contrasting with compound (I), compound (II) is assembled by extensive intermolecular interactions (Table 2). Molecules are linked into inversion dimer–dimer chains through weak C2—H2$A\cdots$O3, C10—H10$B\cdots$O4 and C7—H7$A\cdots$O4 hydrogen bonds, propagating along the [101] direction (Fig. 5). The centrosymmetric dimer formed by the C2—H2$A\cdots$O3 hydrogen-bond pairs generates an $R_2^2(14)$ ring motif. On the other hand, atom O4 serves as a bifurcated acceptor in the $R_1^2(7)$ motif and yet, participates in a second $R_2^2(10)$ ring motif. These dimer–dimer chains are further expanded by C10—H10$A\cdots$O3 and C17—H17$A\cdots$O1 hydrogen bonds through inversion to build a two-dimensional plate parallel to the *ac*-plane (Fig. 6). Within these plates, two kinds of π–π interactions further stabilize the crystal packing: these interactions are between furan rings [centroid–centroid separation: 3.4402 (7) Å; symmetry code: $-x + 1$, $-y + 1$, $-z + 1$] and between a furan ring and a benzene ring [centroid–centroid separation: 3.6088 (7) Å; symmetry code: $-x + 1$, $-y + 1$, $-z + 1$]. In addition, neighboring plates are interconnected *via* C—H$\cdots\pi$ interactions involving the substituted methoxy group and an adjacent phenyl ring (Fig. 7).

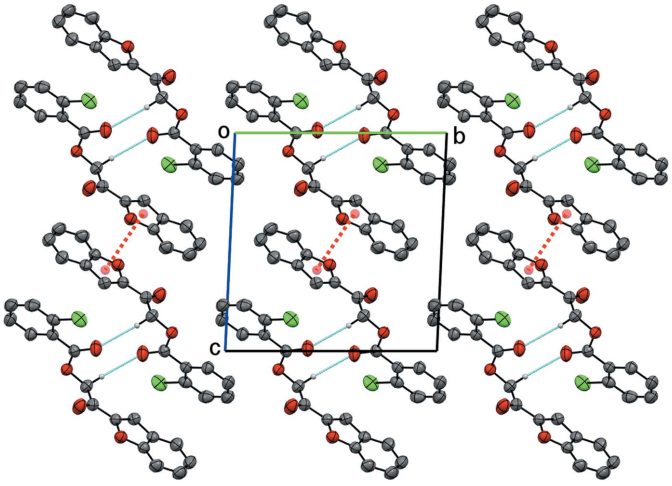


Figure 4
The crystal packing of compound (I), showing hydrogen bonds (cyan dotted lines) and π–π interactions (red dotted lines).

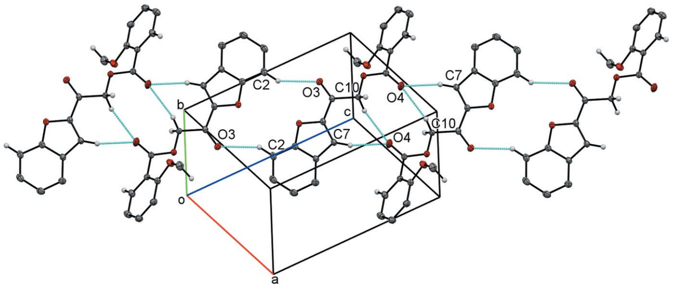


Figure 5
Intermolecular hydrogen bonds joining molecules into an endless chain in compound (II).

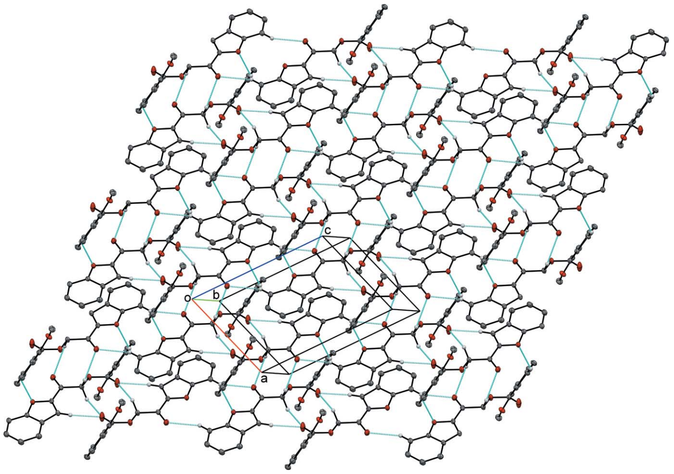


Figure 6
Intermolecular interactions in compound (II), showing the two-dimensional plate parallel to the *ac* plane.

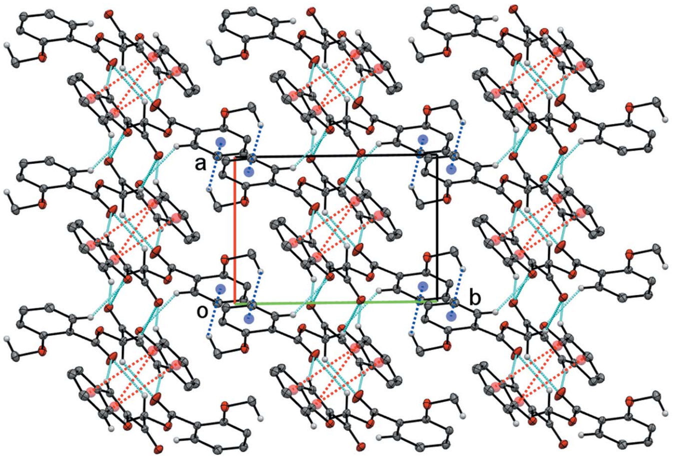


Figure 7
Extensive intermolecular interactions in compound (II), showing hydrogen bonds (cyan dotted lines), C—H$\cdots\pi$ interactions (blue dotted lines) and π–π interactions (red dotted lines).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{17}H_{11}ClO_4$	$C_{18}H_{14}O_5$
M_r	314.71	310.29
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	294	100
a, b, c (Å)	5.5333 (8), 11.3212 (17), 11.5186 (18)	7.4094 (3), 9.7566 (4), 10.5832 (5)
α, β, γ (°)	92.283 (3), 91.536 (3), 99.638 (3)	83.430 (1), 71.808 (1), 87.265 (1)
V (Å^3)	710.41 (19)	721.99 (5)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.28	0.11
Crystal size (mm)	0.54 × 0.25 × 0.21	0.51 × 0.35 × 0.11
Data collection		
Diffractometer	Bruker APEXII DUO CCD area-detector	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.799, 0.944	0.766, 0.950
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12081, 3798, 2860	27838, 4286, 3615
R_{int}	0.026	0.046
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.688	0.708
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.145, 1.03	0.045, 0.124, 1.04
No. of reflections	3798	4286
No. of parameters	199	209
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.27	0.52, −0.33

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *XS* (Sheldrick, 2013), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006) and *PLATON* (Spek, 2009).

4. Database survey

A search of the Cambridge Structural Database (Groom *et al.*, 2016) by using 2-(1-benzofuran-2-yl)-2-oxoethyl benzoate as reference skeleton has revealed five benzofuran structures (Kumar *et al.*, 2015) related to the title compounds, *i.e.* ITAXUY, ITAYAF, ITAYEJ, ITAYIN and ITAYOT. The molecular structures of these compounds differ only at their substituted phenyl rings, especially compound (I) with ITAYAF and compound (II) with ITAYIN, which have the same substituents at altered positions. By looking at their torsion angles at the C—C(═O)—O—C(═O) carbonyl connecting bridge, compound (I) was found to exhibit a *syn*-clinal conformation similar to ITAXUY, ITAYEJ and ITAYIN (τ2 ranges from 75 to 80°) whereas compound (II) shows an *anti*-periplanar conformation as do ITAYAF and ITAYOT (ranging from 163 to 180°).

5. Synthesis and crystallization

The title compounds were synthesized by dissolving a mixture of 1-(benzofuran-2-yl)-2-bromoethan-1-one (1 mmol) with 2-chlorobenzoic acid (1 mmol) for compound (I) and 2-methoxybenzoic acid (1 mmol) for compound (II) in *N*,*N*-dimethylformamide (8 ml). The solution was stirred for about two h at room temperature in the presence of a catalytic amount of anhydrous potassium carbonate and the progress was monitored by thin-layer chromatography (TLC). Once the reaction was complete, the resultant mixture was poured into a beaker of ice cooled water which gave a precipitate. The precipitate obtained was then filtered, washed with distilled water and dried. Finally, pure crystals suitable for X-ray analysis were obtained by slow evaporation using a suitable solvent.

2-(Benzofuran-2-yl)-2-oxoethyl 2-chlorobenzoate (I):

Solvent used to grow crystals: acetone; yield: 79%; m.p. 366–368 K. ^{1}H NMR (500 MHz, CDCl$_3$) in ppm: δ 8.086–8.070 (*d*, 1H, *J* = 7.9 Hz, ^{17}CH), 7.773–7.757 (*d*, 1H, *J* = 7.9 Hz, ^{14}CH), 7.669 (*s*, 1H, ^{7}CH), 7.632–7.615 (*d*, 1H, *J* = 8.4 Hz, ^{2}CH), 7.564–7.530 (*t*, 1H, *J* = 8.4 Hz, ^{3}CH), 7.526–7.510 (*d*, 1H, *J* = 8.4 Hz, ^{5}CH), 7.507–7.474 (*t*, 1H, *J* = 8.4 Hz, ^{4}CH), 7.407–7.355 (*m*, 2H, ^{15}CH, ^{16}CH), 5.595 (*s*, 2H, ^{10}CH$_2$). ^{13}C NMR (125 MHz, CDCl$_3$) in ppm: 183.38 (C9), 164.79 (C11), 155.69 (C1), 150.41 (C8), 134.23 (C12), 133.09 (C15), 132.03 (C16), 131.20 (C3), 129.01 (C6), 128.81 (C14), 126.71 (C5), 126.70 (C4), 124.25 (C13), 123.55 (C17), 113.57 (C7), 112.51 (C2), 66.43 (C10). FT–IR (ATR (solid) cm^{-1}): 3074 (Ar C—H, ν), 2949 (C—H, ν), 1736, 1686 (C═O, ν), 1612 (C═C, ν), 1554, 1472 (Ar C═C, ν), 1255, 1115 (C—O, ν), 1066 (C—Cl, ν).

2-(Benzofuran-2-yl)-2-oxoethyl 2-methoxybenzoate (II):

Solvent used to grow crystals: acetone; yield: 83%; m.p. 378–380 K. ^{1}H NMR (500 MHz, CDCl$_3$) in ppm: δ 8.047–8.032 (*d*, 1H, *J* = 8.0 Hz, ^{17}CH), 7.768–7.752 (*d*, 1H, *J* = 8.0 Hz, ^{14}CH), 7.681 (*s*, 1H, ^{7}CH), 7.636–7.619 (*d*, 1H, *J* = 8.5 Hz, ^{2}CH), 7.569–7.523 (*m*, 2H, ^{5}CH, ^{16}CH), 7.381–7.349 (t, 1H, *J* = 8.0 Hz, ^{15}CH), 7.071–7.033 (*m*, 2H,3CH, ^{4}CH), 5.535 (*s*, 2H, ^{10}CH$_2$), 3.955 (*s*, 3H, ^{18}CH$_3$). ^{13}C NMR (125 MHz, CDCl$_3$) in ppm: 183.98 (C9), 165.18 (C11), 159.68 (C13), 155.66 (C1), 150.55

(C8), 134.22 (C15), 132.33 (C17), 128.68 (C3), 126.77 (C6), 124.15 (C5), 123.48 (C4), 120.26 (C16), 118.80 (C12), 113.57 (C7), 112.53 (C2), 112.10 (C14), 66.09 (C10), 56.05 (C18). FT–IR (ATR (solid) cm^{-1}): 3081 (Ar C—H, ν), 2921 (C—H, ν), 1762, 1686 (C═O, ν), 1601 (C═C, ν), 1554, 1465 (Ar C═C, ν), 1255, 1101 (C—O, ν).

6. Refinement

Crystal data, data collection and structure refinement details are tabulated in Table 3. All C-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å). Refinement was done using a riding model with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C-methyl) and 1.2$U_{\rm eq}$(C) for other H atoms.

Acknowledgements

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supporting information

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Steric repulsion and supramolecular assemblies *via* a two-dimensional plate by C—H···O hydrogen bonds in two closely related 2-(benzofuran-2-yl)-2-oxoethyl benzoates

Li Yee Then, C. S. Chidan Kumar, Huey Chong Kwong, Yip-Foo Win, Siau Hui Mah, Ching Kheng Quah, S. Naveen and Ismail Warad

Computing details

For both structures, data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009). Program(s) used to solve structure: XS (Sheldrick, 2013) for (I); *XS* (Sheldrick, 2013) for (II). Program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) for (I); *SHELXL2013* (Sheldrick, 2015) for (II). For both structures, molecular graphics: *SHELXL2013* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

2-(Benzofuran-2-yl)-2-oxoethyl 2-chlorobenzoate (I)

Crystal data

$C_{17}H_{11}ClO_4$
$M_r = 314.71$
Triclinic, $P\overline{1}$
$a = 5.5333$ (8) Å
$b = 11.3212$ (17) Å
$c = 11.5186$ (18) Å
$\alpha = 92.283$ (3)°
$\beta = 91.536$ (3)°
$\gamma = 99.638$ (3)°
$V = 710.41$ (19) Å^3

$Z = 2$
$F(000) = 324$
$D_x = 1.471$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4675 reflections
$\theta = 2.5–29.0°$
$\mu = 0.28$ mm^{-1}
$T = 294$ K
Block, yellow
0.54 × 0.25 × 0.21 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
$T_{min} = 0.799$, $T_{max} = 0.944$

12081 measured reflections
3798 independent reflections
2860 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 29.3°$, $\theta_{min} = 1.8°$
$h = -7 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.145$
$S = 1.03$
3798 reflections

199 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 0.1547P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Hydrogen site location: inferred from neighbouring sites	$\Delta\rho_{max} = 0.31$ e Å^{-3}
H-atom parameters constrained	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.19628 (9)	0.69545 (5)	1.14636 (5)	0.06498 (18)
O1	0.7395 (2)	0.47462 (10)	0.60559 (10)	0.0487 (3)
O2	0.5749 (2)	0.74445 (10)	0.91565 (10)	0.0472 (3)
O3	0.8481 (3)	0.67643 (12)	0.74537 (13)	0.0669 (4)
O4	0.7470 (3)	0.61109 (11)	1.01203 (13)	0.0651 (4)
C1	0.6380 (3)	0.36403 (15)	0.55782 (13)	0.0451 (4)
C2	0.7437 (4)	0.30006 (18)	0.47427 (16)	0.0595 (5)
H2A	0.8925	0.3303	0.4421	0.071*
C3	0.6141 (5)	0.18868 (19)	0.44183 (18)	0.0683 (6)
H3A	0.6774	0.1419	0.3859	0.082*
C4	0.3920 (5)	0.14375 (18)	0.48973 (18)	0.0653 (5)
H4A	0.3119	0.0673	0.4662	0.078*
C5	0.2876 (4)	0.20964 (17)	0.57136 (17)	0.0579 (4)
H5A	0.1373	0.1796	0.6023	0.069*
C6	0.4152 (3)	0.32335 (14)	0.60635 (13)	0.0443 (4)
C7	0.3768 (3)	0.41575 (15)	0.68858 (14)	0.0450 (4)
H7A	0.2418	0.4159	0.7349	0.054*
C8	0.5753 (3)	0.50274 (14)	0.68559 (13)	0.0429 (3)
C9	0.6496 (3)	0.61413 (14)	0.75465 (14)	0.0459 (4)
C10	0.4630 (3)	0.64691 (15)	0.83864 (15)	0.0489 (4)
H10A	0.3262	0.6698	0.7957	0.059*
H10B	0.4008	0.5781	0.8832	0.059*
C11	0.7212 (3)	0.71241 (14)	1.00006 (14)	0.0438 (3)
C12	0.8368 (3)	0.81814 (14)	1.07463 (13)	0.0419 (3)
C13	1.0492 (3)	0.81829 (16)	1.14281 (14)	0.0465 (4)
C14	1.1527 (4)	0.9200 (2)	1.20965 (16)	0.0601 (5)
H14A	1.2950	0.9196	1.2544	0.072*
C15	1.0459 (4)	1.02112 (19)	1.20989 (17)	0.0638 (5)
H15A	1.1165	1.0892	1.2543	0.077*
C16	0.8358 (4)	1.02186 (17)	1.14495 (17)	0.0619 (5)
H16A	0.7621	1.0899	1.1461	0.074*
C17	0.7331 (4)	0.92144 (15)	1.07765 (16)	0.0515 (4)
H17A	0.5910	0.9232	1.0333	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0480 (3)	0.0749 (3)	0.0767 (3)	0.0207 (2)	−0.0007 (2)	0.0182 (2)
O1	0.0479 (6)	0.0484 (6)	0.0486 (6)	0.0049 (5)	0.0077 (5)	−0.0005 (5)
O2	0.0540 (7)	0.0423 (6)	0.0454 (6)	0.0109 (5)	−0.0056 (5)	−0.0029 (4)
O3	0.0618 (8)	0.0570 (8)	0.0754 (9)	−0.0079 (7)	0.0171 (7)	−0.0119 (6)
O4	0.0736 (9)	0.0398 (6)	0.0813 (9)	0.0112 (6)	−0.0169 (7)	0.0035 (6)
C1	0.0504 (9)	0.0461 (8)	0.0401 (7)	0.0120 (7)	−0.0007 (6)	0.0030 (6)
C2	0.0661 (12)	0.0651 (12)	0.0506 (9)	0.0201 (10)	0.0100 (8)	−0.0007 (8)
C3	0.0932 (16)	0.0647 (12)	0.0519 (10)	0.0311 (12)	0.0006 (10)	−0.0109 (9)
C4	0.0868 (15)	0.0502 (10)	0.0568 (10)	0.0101 (10)	−0.0124 (10)	−0.0096 (8)
C5	0.0612 (11)	0.0530 (10)	0.0554 (10)	0.0001 (8)	−0.0054 (8)	−0.0018 (8)
C6	0.0471 (9)	0.0457 (8)	0.0402 (7)	0.0090 (7)	−0.0036 (6)	0.0019 (6)
C7	0.0427 (8)	0.0485 (9)	0.0435 (8)	0.0071 (7)	0.0015 (6)	0.0000 (6)
C8	0.0449 (8)	0.0439 (8)	0.0405 (7)	0.0096 (6)	0.0019 (6)	0.0022 (6)
C9	0.0478 (9)	0.0426 (8)	0.0466 (8)	0.0053 (7)	0.0010 (7)	0.0020 (6)
C10	0.0497 (9)	0.0476 (9)	0.0480 (8)	0.0072 (7)	−0.0030 (7)	−0.0073 (7)
C11	0.0437 (8)	0.0413 (8)	0.0473 (8)	0.0093 (6)	0.0020 (6)	0.0037 (6)
C12	0.0425 (8)	0.0422 (8)	0.0407 (7)	0.0060 (6)	0.0035 (6)	0.0039 (6)
C13	0.0404 (8)	0.0553 (9)	0.0438 (8)	0.0056 (7)	0.0057 (6)	0.0091 (7)
C14	0.0514 (10)	0.0745 (13)	0.0478 (9)	−0.0070 (9)	−0.0029 (8)	0.0010 (8)
C15	0.0749 (13)	0.0563 (11)	0.0528 (10)	−0.0084 (10)	0.0052 (9)	−0.0070 (8)
C16	0.0786 (14)	0.0459 (10)	0.0604 (11)	0.0097 (9)	0.0077 (10)	−0.0062 (8)
C17	0.0557 (10)	0.0446 (9)	0.0548 (9)	0.0116 (7)	−0.0016 (8)	−0.0009 (7)

Geometric parameters (Å, º)

Cl1—C13	1.7261 (18)	C7—C8	1.349 (2)
O1—C1	1.371 (2)	C7—H7A	0.9300
O1—C8	1.3764 (19)	C8—C9	1.456 (2)
O2—C11	1.3480 (19)	C9—C10	1.514 (2)
O2—C10	1.4328 (19)	C10—H10A	0.9700
O3—C9	1.212 (2)	C10—H10B	0.9700
O4—C11	1.1922 (19)	C11—C12	1.487 (2)
C1—C2	1.382 (2)	C12—C17	1.386 (2)
C1—C6	1.382 (2)	C12—C13	1.396 (2)
C2—C3	1.374 (3)	C13—C14	1.390 (3)
C2—H2A	0.9300	C14—C15	1.373 (3)
C3—C4	1.386 (4)	C14—H14A	0.9300
C3—H3A	0.9300	C15—C16	1.367 (3)
C4—C5	1.375 (3)	C15—H15A	0.9300
C4—H4A	0.9300	C16—C17	1.381 (3)
C5—C6	1.399 (2)	C16—H16A	0.9300
C5—H5A	0.9300	C17—H17A	0.9300
C6—C7	1.429 (2)		
C1—O1—C8	105.45 (12)	C8—C9—C10	115.69 (15)

C11—O2—C10	114.00 (12)	O2—C10—C9	109.79 (14)
O1—C1—C2	125.23 (17)	O2—C10—H10A	109.7
O1—C1—C6	110.63 (14)	C9—C10—H10A	109.7
C2—C1—C6	124.13 (17)	O2—C10—H10B	109.7
C3—C2—C1	115.5 (2)	C9—C10—H10B	109.7
C3—C2—H2A	122.2	H10A—C10—H10B	108.2
C1—C2—H2A	122.2	O4—C11—O2	122.75 (16)
C2—C3—C4	122.16 (19)	O4—C11—C12	126.00 (16)
C2—C3—H3A	118.9	O2—C11—C12	111.24 (13)
C4—C3—H3A	118.9	C17—C12—C13	117.76 (16)
C5—C4—C3	121.47 (19)	C17—C12—C11	119.77 (15)
C5—C4—H4A	119.3	C13—C12—C11	122.48 (14)
C3—C4—H4A	119.3	C14—C13—C12	120.36 (17)
C4—C5—C6	117.8 (2)	C14—C13—Cl1	117.41 (14)
C4—C5—H5A	121.1	C12—C13—Cl1	122.23 (14)
C6—C5—H5A	121.1	C15—C14—C13	120.29 (18)
C1—C6—C5	118.95 (16)	C15—C14—H14A	119.9
C1—C6—C7	105.80 (15)	C13—C14—H14A	119.9
C5—C6—C7	135.22 (17)	C16—C15—C14	120.08 (18)
C8—C7—C6	106.35 (15)	C16—C15—H15A	120.0
C8—C7—H7A	126.8	C14—C15—H15A	120.0
C6—C7—H7A	126.8	C15—C16—C17	119.91 (19)
C7—C8—O1	111.77 (14)	C15—C16—H16A	120.0
C7—C8—C9	131.98 (15)	C17—C16—H16A	120.0
O1—C8—C9	116.14 (14)	C16—C17—C12	121.59 (18)
O3—C9—C8	122.07 (16)	C16—C17—H17A	119.2
O3—C9—C10	122.24 (15)	C12—C17—H17A	119.2

C8—O1—C1—C2	−178.83 (16)	O1—C8—C9—C10	177.42 (13)
C8—O1—C1—C6	0.04 (16)	C11—O2—C10—C9	−76.19 (17)
O1—C1—C2—C3	177.55 (16)	O3—C9—C10—O2	−10.9 (2)
C6—C1—C2—C3	−1.2 (3)	C8—C9—C10—O2	169.07 (13)
C1—C2—C3—C4	0.1 (3)	C10—O2—C11—O4	−2.9 (2)
C2—C3—C4—C5	1.1 (3)	C10—O2—C11—C12	178.34 (13)
C3—C4—C5—C6	−1.1 (3)	O4—C11—C12—C17	−158.19 (18)
O1—C1—C6—C5	−177.75 (14)	O2—C11—C12—C17	20.6 (2)
C2—C1—C6—C5	1.1 (2)	O4—C11—C12—C13	22.0 (3)
O1—C1—C6—C7	0.55 (17)	O2—C11—C12—C13	−159.28 (14)
C2—C1—C6—C7	179.44 (16)	C17—C12—C13—C14	−0.9 (2)
C4—C5—C6—C1	0.0 (2)	C11—C12—C13—C14	178.94 (15)
C4—C5—C6—C7	−177.63 (18)	C17—C12—C13—Cl1	−179.83 (13)
C1—C6—C7—C8	−0.93 (17)	C11—C12—C13—Cl1	0.0 (2)
C5—C6—C7—C8	176.95 (18)	C12—C13—C14—C15	0.5 (3)
C6—C7—C8—O1	1.01 (17)	Cl1—C13—C14—C15	179.46 (15)
C6—C7—C8—C9	−175.02 (16)	C13—C14—C15—C16	0.5 (3)
C1—O1—C8—C7	−0.67 (17)	C14—C15—C16—C17	−1.0 (3)
C1—O1—C8—C9	176.04 (13)	C15—C16—C17—C12	0.6 (3)
C7—C8—C9—O3	173.32 (18)	C13—C12—C17—C16	0.4 (3)

O1—C8—C9—O3	−2.6 (2)	C11—C12—C17—C16	−179.46 (17)
C7—C8—C9—C10	−6.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*B*···O4^i	0.97	2.53	3.495 (2)	176
C17—H17*A*···O2	0.93	2.38	2.700 (2)	100

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

2-(Benzofuran-2-yl)-2-oxoethyl 2-methoxybenzoate (II)

Crystal data

$C_{18}H_{14}O_5$	$Z = 2$
$M_r = 310.29$	$F(000) = 324$
Triclinic, $P\overline{1}$	$D_x = 1.427$ Mg m^{-3}
$a = 7.4094$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.7566$ (4) Å	Cell parameters from 8829 reflections
$c = 10.5832$ (5) Å	$\theta = 2.8$–$30.2°$
$\alpha = 83.430$ (1)°	$\mu = 0.11$ mm^{-1}
$\beta = 71.808$ (1)°	$T = 100$ K
$\gamma = 87.265$ (1)°	Block, colourless
$V = 721.99$ (5) Å^3	0.51 × 0.35 × 0.11 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer	27838 measured reflections
Radiation source: fine-focus sealed tube	4286 independent reflections
Graphite monochromator	3615 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\rm int} = 0.046$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$\theta_{\rm max} = 30.2°$, $\theta_{\rm min} = 2.0°$
$T_{\rm min} = 0.766$, $T_{\rm max} = 0.950$	$h = -10 \rightarrow 10$
	$k = -13 \rightarrow 13$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 0.3014P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{\rm max} = 0.001$
$S = 1.04$	$\Delta\rho_{\rm max} = 0.52$ e Å^{-3}
4286 reflections	$\Delta\rho_{\rm min} = -0.33$ e Å^{-3}
209 parameters	
0 restraints	

Special details

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.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.17733 (11)	0.47109 (8)	0.59014 (8)	0.01564 (17)
O2	0.17204 (12)	0.66894 (8)	0.98339 (8)	0.01707 (18)
O3	0.01605 (12)	0.62351 (9)	0.79953 (8)	0.01888 (18)
O4	0.36010 (15)	0.60784 (11)	1.11020 (10)	0.0314 (2)
O5	0.30167 (13)	0.95091 (9)	0.94102 (8)	0.01990 (19)
C1	0.28755 (15)	0.38063 (11)	0.50676 (11)	0.0145 (2)
C2	0.26141 (17)	0.34956 (13)	0.38921 (11)	0.0190 (2)
H2A	0.1620	0.3901	0.3580	0.023*
C3	0.38996 (18)	0.25537 (13)	0.32014 (12)	0.0215 (2)
H3A	0.3782	0.2302	0.2390	0.026*
C4	0.53699 (18)	0.19608 (13)	0.36640 (12)	0.0224 (2)
H4A	0.6229	0.1326	0.3157	0.027*
C5	0.55911 (17)	0.22858 (13)	0.48483 (12)	0.0198 (2)
H5A	0.6583	0.1878	0.5162	0.024*
C6	0.43110 (15)	0.32313 (11)	0.55666 (11)	0.0146 (2)
C7	0.40703 (16)	0.38347 (11)	0.67825 (11)	0.0149 (2)
H7A	0.4830	0.3667	0.7362	0.018*
C8	0.25361 (15)	0.46946 (11)	0.69393 (10)	0.0142 (2)
C9	0.15814 (15)	0.55579 (11)	0.79978 (11)	0.0142 (2)
C10	0.24468 (16)	0.55128 (11)	0.91227 (11)	0.0151 (2)
H10A	0.2093	0.4650	0.9728	0.018*
H10B	0.3849	0.5548	0.8758	0.018*
C11	0.24999 (15)	0.68820 (12)	1.07844 (11)	0.0153 (2)
C12	0.17567 (15)	0.81458 (11)	1.14463 (11)	0.0142 (2)
C13	0.19740 (15)	0.94584 (12)	1.07249 (11)	0.0153 (2)
C14	0.11950 (16)	1.06035 (12)	1.13868 (12)	0.0180 (2)
H14A	0.1303	1.1496	1.0906	0.022*
C15	0.02584 (17)	1.04355 (13)	1.27532 (12)	0.0206 (2)
H15A	−0.0280	1.1220	1.3198	0.025*
C16	0.00940 (18)	0.91521 (13)	1.34781 (12)	0.0212 (2)
H16A	−0.0537	0.9054	1.4414	0.025*
C17	0.08654 (17)	0.80078 (12)	1.28184 (11)	0.0180 (2)
H17A	0.0782	0.7123	1.3310	0.022*
C18	0.33754 (19)	1.08448 (13)	0.86819 (12)	0.0226 (2)
H18A	0.4241	1.0758	0.7780	0.034*
H18B	0.3955	1.1423	0.9145	0.034*
H18C	0.2176	1.1270	0.8621	0.034*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0172 (4)	0.0179 (4)	0.0137 (4)	0.0017 (3)	−0.0075 (3)	−0.0026 (3)
O2	0.0213 (4)	0.0164 (4)	0.0176 (4)	0.0062 (3)	−0.0112 (3)	−0.0062 (3)
O3	0.0184 (4)	0.0207 (4)	0.0198 (4)	0.0047 (3)	−0.0093 (3)	−0.0037 (3)
O4	0.0403 (6)	0.0307 (5)	0.0362 (5)	0.0198 (4)	−0.0288 (5)	−0.0166 (4)

O5	0.0265 (4)	0.0163 (4)	0.0143 (4)	−0.0002 (3)	−0.0034 (3)	0.0007 (3)
C1	0.0155 (5)	0.0152 (5)	0.0129 (5)	−0.0015 (4)	−0.0046 (4)	−0.0013 (4)
C2	0.0209 (5)	0.0230 (6)	0.0147 (5)	−0.0040 (4)	−0.0075 (4)	−0.0013 (4)
C3	0.0237 (6)	0.0262 (6)	0.0153 (5)	−0.0050 (5)	−0.0053 (4)	−0.0056 (4)
C4	0.0234 (6)	0.0234 (6)	0.0201 (6)	0.0007 (4)	−0.0041 (4)	−0.0086 (4)
C5	0.0197 (5)	0.0202 (5)	0.0201 (5)	0.0025 (4)	−0.0065 (4)	−0.0046 (4)
C6	0.0167 (5)	0.0141 (5)	0.0129 (5)	−0.0006 (4)	−0.0048 (4)	−0.0007 (4)
C7	0.0180 (5)	0.0147 (5)	0.0128 (5)	0.0001 (4)	−0.0063 (4)	−0.0004 (4)
C8	0.0165 (5)	0.0146 (5)	0.0125 (5)	−0.0009 (4)	−0.0062 (4)	−0.0005 (4)
C9	0.0161 (5)	0.0136 (5)	0.0133 (5)	−0.0012 (4)	−0.0053 (4)	−0.0003 (4)
C10	0.0184 (5)	0.0151 (5)	0.0132 (5)	0.0041 (4)	−0.0068 (4)	−0.0035 (4)
C11	0.0164 (5)	0.0163 (5)	0.0145 (5)	0.0012 (4)	−0.0070 (4)	−0.0017 (4)
C12	0.0155 (5)	0.0140 (5)	0.0144 (5)	0.0012 (4)	−0.0065 (4)	−0.0025 (4)
C13	0.0158 (5)	0.0166 (5)	0.0143 (5)	0.0006 (4)	−0.0061 (4)	−0.0014 (4)
C14	0.0198 (5)	0.0146 (5)	0.0206 (5)	0.0015 (4)	−0.0076 (4)	−0.0023 (4)
C15	0.0205 (5)	0.0193 (5)	0.0225 (6)	0.0013 (4)	−0.0059 (4)	−0.0072 (4)
C16	0.0231 (5)	0.0235 (6)	0.0153 (5)	−0.0011 (4)	−0.0023 (4)	−0.0050 (4)
C17	0.0207 (5)	0.0172 (5)	0.0160 (5)	−0.0018 (4)	−0.0056 (4)	−0.0008 (4)
C18	0.0278 (6)	0.0190 (5)	0.0197 (5)	−0.0041 (4)	−0.0072 (5)	0.0042 (4)

Geometric parameters (Å, º)

O1—C1	1.3726 (13)	C7—H7A	0.9500
O1—C8	1.3817 (13)	C8—C9	1.4591 (15)
O2—C11	1.3405 (13)	C9—C10	1.5141 (15)
O2—C10	1.4352 (13)	C10—H10A	0.9900
O3—C9	1.2165 (13)	C10—H10B	0.9900
O4—C11	1.2013 (14)	C11—C12	1.4854 (15)
O5—C13	1.3608 (13)	C12—C17	1.3885 (15)
O5—C18	1.4278 (14)	C12—C13	1.4029 (15)
C1—C2	1.3854 (15)	C13—C14	1.3918 (15)
C1—C6	1.3968 (15)	C14—C15	1.3891 (17)
C2—C3	1.3862 (17)	C14—H14A	0.9500
C2—H2A	0.9500	C15—C16	1.3811 (17)
C3—C4	1.4033 (18)	C15—H15A	0.9500
C3—H3A	0.9500	C16—C17	1.3888 (16)
C4—C5	1.3865 (17)	C16—H16A	0.9500
C4—H4A	0.9500	C17—H17A	0.9500
C5—C6	1.3983 (15)	C18—H18A	0.9800
C5—H5A	0.9500	C18—H18B	0.9800
C6—C7	1.4333 (15)	C18—H18C	0.9800
C7—C8	1.3589 (15)		
C1—O1—C8	105.39 (8)	C9—C10—H10A	110.3
C11—O2—C10	114.70 (8)	O2—C10—H10B	110.3
C13—O5—C18	116.85 (9)	C9—C10—H10B	110.3
O1—C1—C2	125.19 (10)	H10A—C10—H10B	108.5
O1—C1—C6	110.64 (9)	O4—C11—O2	123.18 (11)

C2—C1—C6	124.16 (11)	O4—C11—C12	124.35 (10)
C1—C2—C3	115.56 (11)	O2—C11—C12	112.37 (9)
C1—C2—H2A	122.2	C17—C12—C13	120.00 (10)
C3—C2—H2A	122.2	C17—C12—C11	118.36 (10)
C2—C3—C4	122.01 (11)	C13—C12—C11	121.63 (10)
C2—C3—H3A	119.0	O5—C13—C14	124.76 (10)
C4—C3—H3A	119.0	O5—C13—C12	115.95 (10)
C5—C4—C3	121.16 (11)	C14—C13—C12	119.25 (10)
C5—C4—H4A	119.4	C15—C14—C13	119.68 (11)
C3—C4—H4A	119.4	C15—C14—H14A	120.2
C4—C5—C6	118.01 (11)	C13—C14—H14A	120.2
C4—C5—H5A	121.0	C16—C15—C14	121.37 (11)
C6—C5—H5A	121.0	C16—C15—H15A	119.3
C1—C6—C5	119.09 (10)	C14—C15—H15A	119.3
C1—C6—C7	105.80 (9)	C15—C16—C17	119.02 (11)
C5—C6—C7	135.10 (11)	C15—C16—H16A	120.5
C8—C7—C6	106.09 (9)	C17—C16—H16A	120.5
C8—C7—H7A	127.0	C12—C17—C16	120.59 (11)
C6—C7—H7A	127.0	C12—C17—H17A	119.7
C7—C8—O1	112.07 (9)	C16—C17—H17A	119.7
C7—C8—C9	131.43 (10)	O5—C18—H18A	109.5
O1—C8—C9	116.50 (9)	O5—C18—H18B	109.5
O3—C9—C8	122.38 (10)	H18A—C18—H18B	109.5
O3—C9—C10	122.39 (10)	O5—C18—H18C	109.5
C8—C9—C10	115.20 (9)	H18A—C18—H18C	109.5
O2—C10—C9	107.13 (8)	H18B—C18—H18C	109.5
O2—C10—H10A	110.3		

C8—O1—C1—C2	179.76 (10)	C11—O2—C10—C9	−173.51 (9)
C8—O1—C1—C6	−0.15 (12)	O3—C9—C10—O2	−18.82 (14)
O1—C1—C2—C3	179.82 (10)	C8—C9—C10—O2	163.15 (9)
C6—C1—C2—C3	−0.28 (17)	C10—O2—C11—O4	−6.03 (17)
C1—C2—C3—C4	−0.22 (17)	C10—O2—C11—C12	177.51 (9)
C2—C3—C4—C5	0.57 (19)	O4—C11—C12—C17	−55.50 (17)
C3—C4—C5—C6	−0.42 (18)	O2—C11—C12—C17	120.91 (11)
O1—C1—C6—C5	−179.67 (10)	O4—C11—C12—C13	123.09 (14)
C2—C1—C6—C5	0.42 (17)	O2—C11—C12—C13	−60.51 (14)
O1—C1—C6—C7	−0.36 (12)	C18—O5—C13—C14	2.08 (16)
C2—C1—C6—C7	179.73 (10)	C18—O5—C13—C12	−175.45 (10)
C4—C5—C6—C1	−0.05 (17)	C17—C12—C13—O5	174.12 (10)
C4—C5—C6—C7	−179.11 (12)	C11—C12—C13—O5	−4.45 (15)
C1—C6—C7—C8	0.73 (12)	C17—C12—C13—C14	−3.55 (16)
C5—C6—C7—C8	179.88 (13)	C11—C12—C13—C14	177.88 (10)
C6—C7—C8—O1	−0.87 (12)	O5—C13—C14—C15	−175.85 (11)
C6—C7—C8—C9	178.16 (11)	C12—C13—C14—C15	1.60 (17)
C1—O1—C8—C7	0.65 (12)	C13—C14—C15—C16	0.55 (18)
C1—O1—C8—C9	−178.54 (9)	C14—C15—C16—C17	−0.74 (19)
C7—C8—C9—O3	−177.25 (11)	C13—C12—C17—C16	3.40 (17)

O1—C8—C9—O3	1.74 (16)	C11—C12—C17—C16	−177.99 (10)
C7—C8—C9—C10	0.77 (17)	C15—C16—C17—C12	−1.25 (18)
O1—C8—C9—C10	179.77 (9)		

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O3^{i}	0.95	2.45	3.2677 (15)	145
C7—H7*A*···O4^{ii}	0.95	2.31	3.2352 (16)	163
C10—H10*A*···O3^{iii}	0.99	2.55	3.3746 (14)	141
C10—H10*B*···O4^{ii}	0.99	2.44	3.2028 (17)	134
C17—H17*A*···O1^{iii}	0.95	2.55	3.2730 (15)	134
C18—H18*C*···*Cg*3^{iv}	0.98	2.81	3.6181 (16)	141

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*, −*y*+1, −*z*+2; (iv) −*x*, −*y*+2, −*z*+2.

π–π interactions in compound (II).

Centroid 1	Centroid 2	Centroid-to-centroid distance (Å)	Symmetry code
*Cg*1	*Cg*1	3.4402 (7)	-x+1, -y+1, -z+1
*Cg*1	*Cg*2	3.6088 (7)	-x+1, -y+1, -z+1

*Cg*1 and *Cg*2 are the centroids of O1/C1/C6/C7/C8 and C1–C6 rings, respectively.