

2-(4-Methylphenyl)-7-(2-methylpropoxy)-4*H*-chromen-4-one–6-chloro-2-(4-methylphenyl)-7-(2-methylpropoxy)-4*H*-chromen-4-one (19/1)

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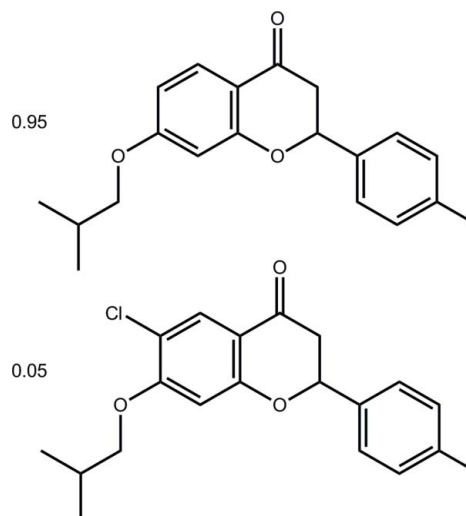
Received 19 June 2012; accepted 24 July 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 17.6.

The title co-crystal, $0.95\text{C}_{20}\text{H}_{20}\text{O}_3 \cdot 0.05\text{C}_{20}\text{H}_{19}\text{ClO}_3$, arises as the chloride carried over during the synthesis shares a position with an aromatic H atom; the partial occupancies are 0.947 (2) and 0.053 (2) for H and Cl, respectively. The molecular structure is stabilized by intramolecular $\text{C}-\text{H} \cdots \text{O}$ contacts, forming pseudo five- and six-membered rings with $S(5)$ and $S(6)$ graph-set motifs, respectively. The crystal structure features $\pi-\pi$ stacking interactions between the centroids of the central fused ring systems [centroid–centroid distance = 3.501 (2) Å].

Related literature

For background to flavones, see: Hollman *et al.* (1997); Yao *et al.* (2004). For the biological activity of flavones, see: Harborne & Williams (2000); Khan & Hasan (2003); Qin *et al.* (2008); Mota *et al.* (2009); Prakash *et al.* (2009). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$0.95\text{C}_{20}\text{H}_{20}\text{O}_3 \cdot 0.05\text{C}_{20}\text{H}_{19}\text{ClO}_3$
 $M_r = 310.19$
 Triclinic, $P\bar{1}$
 $a = 9.0371$ (2) Å
 $b = 9.6216$ (2) Å
 $c = 11.0308$ (3) Å
 $\alpha = 75.171$ (2)°
 $\beta = 65.865$ (2)°

$\gamma = 69.833$ (1)°
 $V = 814.20$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2004)
 $T_{\min} = 0.973$, $T_{\max} = 0.982$

18174 measured reflections
 3847 independent reflections
 2737 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.136$
 $S = 1.06$
 3847 reflections

219 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{C}19-\text{H}19 \cdots \text{O}3$	0.93	2.38	2.702 (2)	100
$\text{Cl}1-\text{H}1A \cdots \text{O}1$	0.96	2.58	2.900 (2)	100

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT (Bruker, 2004); data reduction: SAINT and XPREP (Bruker, 2004); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5116).

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supporting information

Acta Cryst. (2012). E68, o2582–o2583 [https://doi.org/10.1107/S1600536812033430]

2-(4-Methylphenyl)-7-(2-methylpropoxy)-4*H*-chromen-4-one–6-chloro-2-(4-methylphenyl)-7-(2-methylpropoxy)-4*H*-chromen-4-one (19/1)

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S1. Comment

Flavones can be considered as the derivatives of a parent compound 2-phenylchromen containing varying degrees of hydroxylation and methoxylation (Yao *et al.*, 2004). Also, flavones and their derivatives at different oxidation level are well known naturally occurring oxygen-containing potent anti-oxidant heterocyclic compounds as they chelate ions, scavenge oxygen free radicals and prevent the oxidation of low density lipoprotein (Hollman *et al.*, 1997). Both natural and synthetic flavones possess a wide spectrum of biological activities such as anti-bacterial, anti-fungal, anti-inflammatory, anti-cancer, *etc.* (Prakash *et al.*, 2009; Mota *et al.*, 2009; Qin *et al.*, 2008; Khan & Hasan, 2003). The continuous search for the synthesis of new derivatives in this group due to their medicinal importance (Harborne & Williams, 2000) is the main motivation for the study of title flavone molecule. In view of their importance, the title compound, 2-(4-methylphenyl)-7-(2-methylpropoxy)-4*H*-chromen-4-one (I) was synthesized and its crystal structure studied.

The molecular structure of (I), Fig. 1, consists of a central chromen ring extended by a toluene ring on one side and a propoxy moiety on other side. The bicyclic chromen ring is almost coplanar with C8, C12 and C13 atoms have maximum respective deviations of -0.205 (16), 0.0185 (16) and 0.158 (15) Å with respect to least square plane through it. The fractional chlorine atom remains in the molecule of (I) during the synthesis and its presence is confirmed during the structural refinement as it shares a position with the aromatic hydrogen H19 atom; the partial occupancies are 0.947 (2) and 0.053 (2) for H19 and Cl1 atoms, respectively. In the absence of hydrogen bonds, the crystal structure of (I) is stabilized by intramolecular short C—H...O contacts forming pseudo five- and six-membered rings of *S*(5) and *S*(6) graph-set motif (Bernstein *et al.*, 1995), Table 1, and by π — π stacking interactions between symmetry related fused chromen rings ($Cg1-Cg2$ ($2-x, -y, 1-z$) = 3.501 (2) Å; $Cg1 = C5-C10$ and $Cg2 = O3/C9/C8/C11-C13$), Fig. 2.

S2. Experimental

(2*E*)-1-[2-Hydroxy-4-(2-methylpropoxy)phenyl]-3-(4-methylphenyl)prop-2-ene-1-one (0.01 mol) was dissolved in DMSO (30 ml) and iodine, in crystalline powder form, was added. The mixture was then heated at about 140–145 °C for 1 h and the reaction was monitored by continuous TLC. The resulting solution was cooled and diluted with water after the completion of reaction. Excess iodine was removed by filtering and washing the product with 20% aqueous sodium bisulphite. The crude product was then purified by column chromatography using toluene-ethyl acetate (10:1) as the mobile phase and a silica gel as the stationary phase. The melting point was measured on an Electro thermal 9200 apparatus and is uncorrected (Yield: 68%, *M.pt*: 442 K). The colourless block-shaped crystals of the title compound were obtained by re-crystallization from its ethanol solution.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions ($C-H = 0.93$ to 0.98 Å) and were included in the refinement in the riding model approximation with $U_{iso}(H)$ set to $1.2-1.5U_{eq}(C)$. A reflection affected by the beam stop, *i.e.* (0 0 1), was omitted from the final refinement.

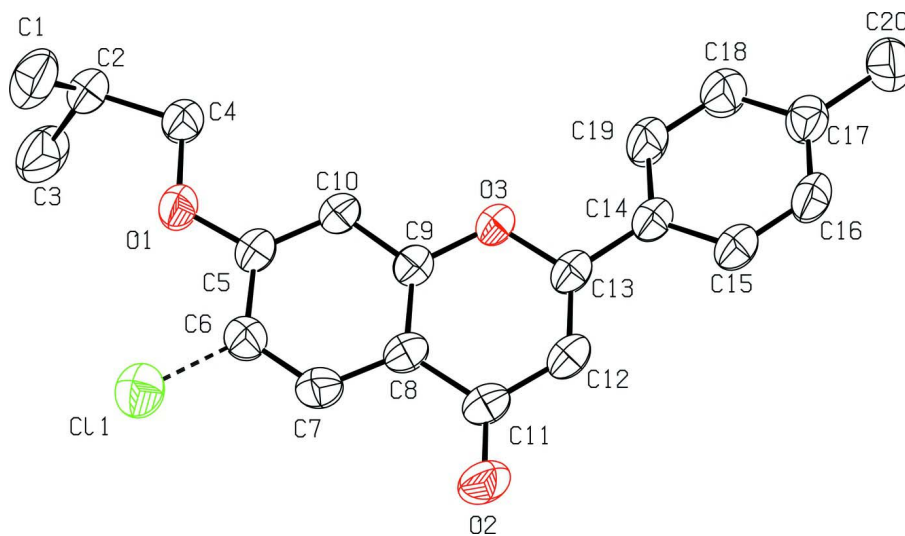


Figure 1

Molecular structure of (I) showing 50% probability displacement ellipsoids. The hydrogen atoms are omitted for clarity.

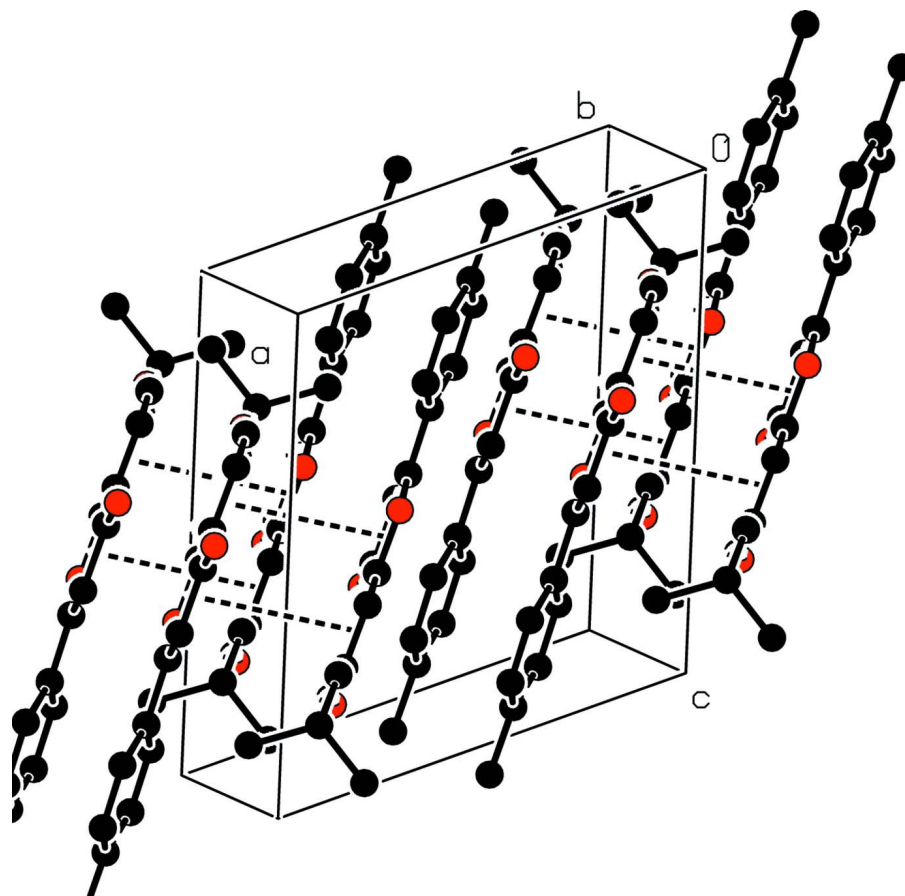


Figure 2

Crystal packing showing π — π stacking interactions indicated by dashed lines. H atoms are omitted for clarity.

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Crystal data

$0.95\text{C}_{20}\text{H}_{20}\text{O}_3 \cdot 0.05\text{C}_{20}\text{H}_{19}\text{ClO}_3$

$M_r = 310.19$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 9.0371(2) \text{ \AA}$

$b = 9.6216(2) \text{ \AA}$

$c = 11.0308(3) \text{ \AA}$

$\alpha = 75.171(2)^\circ$

$\beta = 65.865(2)^\circ$

$\gamma = 69.833(1)^\circ$

$V = 814.20(4) \text{ \AA}^3$

$Z = 2$

$F(000) = 329.6$

$D_x = 1.265 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 5339 reflections

$\theta = 3.0\text{--}25.0^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.30 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and φ scan

Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)

$T_{\min} = 0.973$, $T_{\max} = 0.982$

18174 measured reflections

3847 independent reflections

2737 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 27.8^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$h = -11 \rightarrow 11$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.136$
 $S = 1.06$
 3847 reflections
 219 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
 $w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.1669P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.005$
 $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Special details

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.96616 (14)	-0.37259 (11)	0.75225 (11)	0.0496 (3)	
O2	0.73241 (16)	0.33677 (12)	0.64615 (12)	0.0611 (3)	
O3	0.72302 (13)	0.01688 (10)	0.47020 (10)	0.0427 (3)	
C1	0.9533 (3)	-0.6722 (2)	0.8857 (2)	0.0753 (6)	
H1B	1.0079	-0.7685	0.9223	0.113*	
H1C	0.8465	-0.6739	0.8881	0.113*	
H1A	0.9360	-0.5981	0.9377	0.113*	
C2	1.0620 (2)	-0.63483 (17)	0.74312 (17)	0.0502 (4)	
H2	1.0725	-0.7099	0.6924	0.060*	
C3	1.2383 (2)	-0.6446 (2)	0.7309 (3)	0.0807 (7)	
H3C	1.3039	-0.6216	0.6384	0.121*	
H3A	1.2900	-0.7440	0.7645	0.121*	
H3B	1.2327	-0.5746	0.7820	0.121*	
C4	0.9825 (2)	-0.48407 (16)	0.67936 (16)	0.0464 (4)	
H4A	1.0526	-0.4655	0.5862	0.056*	
H4B	0.8726	-0.4815	0.6828	0.056*	
C5	0.90580 (18)	-0.22724 (16)	0.70937 (15)	0.0412 (3)	
C6	0.9127 (2)	-0.12487 (17)	0.77583 (16)	0.0471 (4)	
H6	0.9567	-0.1590	0.8443	0.057*	0.9470 (18)
C7	0.8550 (2)	0.02482 (17)	0.74021 (16)	0.0467 (4)	
H7	0.8601	0.0919	0.7851	0.056*	
C8	0.78841 (17)	0.07948 (16)	0.63740 (14)	0.0398 (3)	

C9	0.78410 (17)	-0.02488 (15)	0.57358 (14)	0.0373 (3)	
C10	0.84152 (17)	-0.17760 (15)	0.60726 (14)	0.0397 (3)	
H10	0.8369	-0.2447	0.5623	0.048*	
C11	0.72965 (19)	0.23849 (16)	0.59441 (15)	0.0446 (4)	
C12	0.67062 (19)	0.27121 (16)	0.48452 (16)	0.0455 (4)	
H12	0.6314	0.3707	0.4520	0.055*	
C13	0.66968 (17)	0.16449 (15)	0.42691 (15)	0.0406 (3)	
C14	0.61702 (18)	0.18806 (16)	0.31181 (15)	0.0425 (3)	
C15	0.5271 (2)	0.32770 (17)	0.26928 (16)	0.0485 (4)	
H15	0.4986	0.4081	0.3142	0.058*	
C16	0.4797 (2)	0.34794 (17)	0.16082 (17)	0.0507 (4)	
H16	0.4203	0.4427	0.1334	0.061*	
C17	0.5174 (2)	0.23220 (18)	0.09144 (16)	0.0489 (4)	
C18	0.6088 (3)	0.09398 (19)	0.13338 (19)	0.0627 (5)	
H18	0.6381	0.0141	0.0877	0.075*	
C19	0.6579 (2)	0.07170 (18)	0.24164 (19)	0.0587 (5)	
H19	0.7191	-0.0227	0.2678	0.070*	
C20	0.4595 (2)	0.2551 (2)	-0.02344 (18)	0.0628 (5)	
H20A	0.5374	0.2937	-0.1039	0.094*	
H20B	0.3498	0.3249	-0.0052	0.094*	
H20C	0.4543	0.1615	-0.0348	0.094*	
Cl1	0.9913 (10)	-0.1791 (10)	0.9090 (9)	0.060 (3)	0.0530 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0659 (7)	0.0342 (6)	0.0515 (7)	-0.0061 (5)	-0.0312 (6)	-0.0029 (5)
O2	0.0839 (9)	0.0380 (6)	0.0665 (8)	-0.0159 (6)	-0.0280 (7)	-0.0138 (5)
O3	0.0506 (6)	0.0282 (5)	0.0497 (6)	-0.0065 (4)	-0.0231 (5)	-0.0029 (4)
C1	0.1004 (16)	0.0513 (11)	0.0633 (12)	-0.0210 (11)	-0.0291 (12)	0.0109 (9)
C2	0.0599 (10)	0.0339 (8)	0.0580 (10)	-0.0101 (7)	-0.0277 (8)	-0.0004 (7)
C3	0.0635 (12)	0.0462 (10)	0.132 (2)	-0.0063 (9)	-0.0503 (13)	0.0042 (11)
C4	0.0549 (9)	0.0370 (8)	0.0483 (9)	-0.0088 (7)	-0.0225 (7)	-0.0050 (7)
C5	0.0415 (8)	0.0339 (7)	0.0433 (8)	-0.0072 (6)	-0.0135 (7)	-0.0037 (6)
C6	0.0529 (9)	0.0455 (9)	0.0457 (9)	-0.0121 (7)	-0.0212 (7)	-0.0062 (7)
C7	0.0517 (9)	0.0428 (9)	0.0487 (9)	-0.0137 (7)	-0.0164 (7)	-0.0121 (7)
C8	0.0381 (7)	0.0348 (7)	0.0422 (8)	-0.0108 (6)	-0.0075 (6)	-0.0079 (6)
C9	0.0356 (7)	0.0344 (7)	0.0382 (8)	-0.0092 (6)	-0.0102 (6)	-0.0039 (6)
C10	0.0424 (8)	0.0325 (7)	0.0428 (8)	-0.0091 (6)	-0.0142 (7)	-0.0055 (6)
C11	0.0455 (8)	0.0356 (8)	0.0477 (9)	-0.0117 (6)	-0.0086 (7)	-0.0099 (6)
C12	0.0479 (9)	0.0287 (7)	0.0521 (9)	-0.0057 (6)	-0.0146 (7)	-0.0045 (6)
C13	0.0376 (7)	0.0305 (7)	0.0459 (8)	-0.0066 (6)	-0.0111 (6)	-0.0021 (6)
C14	0.0424 (8)	0.0321 (7)	0.0478 (9)	-0.0083 (6)	-0.0149 (7)	-0.0010 (6)
C15	0.0510 (9)	0.0331 (8)	0.0560 (10)	-0.0065 (7)	-0.0190 (8)	-0.0040 (7)
C16	0.0494 (9)	0.0361 (8)	0.0589 (10)	-0.0077 (7)	-0.0224 (8)	0.0062 (7)
C17	0.0473 (9)	0.0475 (9)	0.0483 (9)	-0.0161 (7)	-0.0169 (7)	0.0039 (7)
C18	0.0868 (13)	0.0410 (9)	0.0661 (12)	-0.0078 (9)	-0.0392 (11)	-0.0094 (8)
C19	0.0780 (12)	0.0320 (8)	0.0685 (11)	0.0000 (8)	-0.0408 (10)	-0.0060 (7)

C20	0.0691 (12)	0.0642 (12)	0.0582 (11)	-0.0207 (9)	-0.0303 (9)	0.0033 (9)
C11	0.053 (5)	0.061 (6)	0.059 (5)	-0.016 (4)	-0.016 (4)	-0.001 (4)

Geometric parameters (Å, °)

O1—C5	1.3503 (17)	C7—H7	0.9300
O1—C4	1.4333 (17)	C8—C9	1.3844 (19)
O2—C11	1.2348 (17)	C8—C11	1.457 (2)
O3—C13	1.3589 (16)	C9—C10	1.3852 (19)
O3—C9	1.3762 (17)	C10—H10	0.9300
C1—C2	1.503 (3)	C11—C12	1.439 (2)
C1—H1B	0.9600	C12—C13	1.343 (2)
C1—H1C	0.9600	C12—H12	0.9300
C1—H1A	0.9600	C13—C14	1.470 (2)
C2—C4	1.513 (2)	C14—C19	1.383 (2)
C2—C3	1.514 (2)	C14—C15	1.386 (2)
C2—H2	0.9800	C15—C16	1.377 (2)
C3—H3C	0.9600	C15—H15	0.9300
C3—H3A	0.9600	C16—C17	1.380 (2)
C3—H3B	0.9600	C16—H16	0.9300
C4—H4A	0.9700	C17—C18	1.380 (2)
C4—H4B	0.9700	C17—C20	1.499 (2)
C5—C10	1.379 (2)	C18—C19	1.380 (2)
C5—C6	1.401 (2)	C18—H18	0.9300
C6—C7	1.364 (2)	C19—H19	0.9300
C6—C11	1.772 (9)	C20—H20A	0.9600
C6—H6	0.9300	C20—H20B	0.9600
C7—C8	1.400 (2)	C20—H20C	0.9600
C5—O1—C4	118.87 (11)	O3—C9—C8	121.81 (12)
C13—O3—C9	119.23 (11)	O3—C9—C10	115.07 (12)
C2—C1—H1B	109.5	C8—C9—C10	123.12 (13)
C2—C1—H1C	109.5	C5—C10—C9	118.11 (13)
H1B—C1—H1C	109.5	C5—C10—H10	120.9
C2—C1—H1A	109.5	C9—C10—H10	120.9
H1B—C1—H1A	109.5	O2—C11—C12	122.81 (14)
H1C—C1—H1A	109.5	O2—C11—C8	123.12 (14)
C1—C2—C4	112.08 (15)	C12—C11—C8	114.06 (12)
C1—C2—C3	112.10 (17)	C13—C12—C11	122.91 (13)
C4—C2—C3	110.95 (14)	C13—C12—H12	118.5
C1—C2—H2	107.1	C11—C12—H12	118.5
C4—C2—H2	107.1	C12—C13—O3	121.86 (13)
C3—C2—H2	107.1	C12—C13—C14	126.37 (13)
C2—C3—H3C	109.5	O3—C13—C14	111.77 (12)
C2—C3—H3A	109.5	C19—C14—C15	118.04 (14)
H3C—C3—H3A	109.5	C19—C14—C13	120.87 (13)
C2—C3—H3B	109.5	C15—C14—C13	121.09 (14)
H3C—C3—H3B	109.5	C16—C15—C14	120.31 (14)

H3A—C3—H3B	109.5	C16—C15—H15	119.8
O1—C4—C2	107.95 (12)	C14—C15—H15	119.8
O1—C4—H4A	110.1	C15—C16—C17	122.14 (14)
C2—C4—H4A	110.1	C15—C16—H16	118.9
O1—C4—H4B	110.1	C17—C16—H16	118.9
C2—C4—H4B	110.1	C16—C17—C18	117.17 (15)
H4A—C4—H4B	108.4	C16—C17—C20	121.40 (15)
O1—C5—C10	124.33 (13)	C18—C17—C20	121.43 (16)
O1—C5—C6	115.33 (13)	C19—C18—C17	121.49 (16)
C10—C5—C6	120.34 (13)	C19—C18—H18	119.3
C7—C6—C5	120.05 (14)	C17—C18—H18	119.3
C7—C6—C11	116.7 (3)	C18—C19—C14	120.84 (15)
C5—C6—C11	123.2 (3)	C18—C19—H19	119.6
C7—C6—H6	120.0	C14—C19—H19	119.6
C5—C6—H6	120.0	C17—C20—H20A	109.5
C6—C7—C8	121.26 (13)	C17—C20—H20B	109.5
C6—C7—H7	119.4	H20A—C20—H20B	109.5
C8—C7—H7	119.4	C17—C20—H20C	109.5
C9—C8—C7	117.11 (13)	H20A—C20—H20C	109.5
C9—C8—C11	120.11 (13)	H20B—C20—H20C	109.5
C7—C8—C11	122.75 (13)		
C5—O1—C4—C2	176.62 (13)	C7—C8—C11—O2	-0.8 (2)
C1—C2—C4—O1	62.80 (18)	C9—C8—C11—C12	0.0 (2)
C3—C2—C4—O1	-63.37 (19)	C7—C8—C11—C12	178.16 (14)
C4—O1—C5—C10	7.0 (2)	O2—C11—C12—C13	179.05 (15)
C4—O1—C5—C6	-172.61 (13)	C8—C11—C12—C13	0.1 (2)
O1—C5—C6—C7	179.97 (14)	C11—C12—C13—O3	0.9 (2)
C10—C5—C6—C7	0.3 (2)	C11—C12—C13—C14	-177.83 (14)
O1—C5—C6—C11	-1.0 (4)	C9—O3—C13—C12	-1.8 (2)
C10—C5—C6—C11	179.3 (3)	C9—O3—C13—C14	177.06 (12)
C5—C6—C7—C8	-0.1 (2)	C12—C13—C14—C19	164.68 (16)
C11—C6—C7—C8	-179.2 (3)	O3—C13—C14—C19	-14.1 (2)
C6—C7—C8—C9	-0.1 (2)	C12—C13—C14—C15	-14.5 (2)
C6—C7—C8—C11	-178.39 (14)	O3—C13—C14—C15	166.74 (13)
C13—O3—C9—C8	1.8 (2)	C19—C14—C15—C16	0.4 (2)
C13—O3—C9—C10	-177.59 (12)	C13—C14—C15—C16	179.60 (14)
C7—C8—C9—O3	-179.21 (13)	C14—C15—C16—C17	0.6 (2)
C11—C8—C9—O3	-0.9 (2)	C15—C16—C17—C18	-1.4 (2)
C7—C8—C9—C10	0.2 (2)	C15—C16—C17—C20	177.83 (15)
C11—C8—C9—C10	178.47 (13)	C16—C17—C18—C19	1.2 (3)
O1—C5—C10—C9	-179.90 (13)	C20—C17—C18—C19	-178.04 (17)
C6—C5—C10—C9	-0.3 (2)	C17—C18—C19—C14	-0.2 (3)
O3—C9—C10—C5	179.46 (12)	C15—C14—C19—C18	-0.6 (3)
C8—C9—C10—C5	0.0 (2)	C13—C14—C19—C18	-179.81 (16)
C9—C8—C11—O2	-179.02 (14)		

Hydrogen-bond geometry (Å, °)

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C19—H19···O3	0.93	2.38	2.702 (2)	100
C1—H1A···O1	0.96	2.58	2.900 (2)	100