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(*Z*)-Methyl 2-[(4-bromo-2-formylphenoxy)methyl]-3-*o*-tolylacrylate

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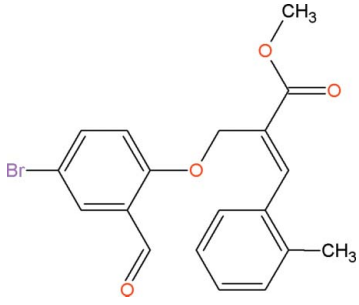
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.125; data-to-parameter ratio = 24.8.

In the title compound, $C_{19}H_{17}BrO_4$, the dihedral angle between the two benzene rings is 82.1 (1)°. The molecular structure is stabilized by an intramolecular C—H···O hydrogen bond which generates an S(7) ring motif. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds and C—H···π interactions. Intermolecular C—H···O interactions are involved in the formation of centrosymmetric $R_2^2(16)$ dimers, which are connected into supramolecular tapes running along the [100] direction.

Related literature

For background to the applications of acrylates, see: de Fraine *et al.* (1991); Zhang & Ji (1992). For related structures, see: Wang *et al.* (2011); Hou (2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{17}BrO_4$
M_r = 389.24
Triclinic, $P\overline{1}$
a = 8.0114 (2) Å
b = 8.6138 (2) Å
c = 13.4827 (4) Å
α = 96.466 (1)°
β = 97.185 (1)°
γ = 106.546 (2)°
V = 874.08 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.37 mm^{-1}
T = 293 K
0.25 × 0.23 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.547, T_{max} = 0.653
21788 measured reflections
5440 independent reflections
2870 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
S = 1.02
5440 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

Cg is the centroid of the C13–C18 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O3	0.93	2.59	3.377 (3)	143
C19—H19B···O1^{i}	0.96	2.53	3.436 (3)	157
C5—H5···O4^{ii}	0.93	2.44	3.273 (3)	149
C19—H19C···Cg^{iii}	0.96	2.74	3.580 (3)	147

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

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: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

SM thanks Dr Babu Vargheese, SAIF, IIT, Madras, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5640).

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supporting information

Acta Cryst. (2011). E**67**, o2690 [https://doi.org/10.1107/S1600536811037731]

(*Z*)-Methyl 2-[(4-bromo-2-formylphenoxy)methyl]-3-*o*-tolylacrylate

S. Vijayakumar, R. Madhanraj, S. Murugavel, R. Selvakumar and M. Bakthadoss

S1. Comment

Acrylate and its derivatives are important compounds because of their agrochemical and medical applications (de Fraine *et al.,* 1991; Zhang & Ji, 1992).

Fig. 1. shows a displacement ellipsoid plot of the title compound with the atom numbering scheme. The dihedral angle between the two aromatic rings is 82.1 (1)°. The methyl acrylate (O1/O2/C7-C10) plane forms dihedral angles of 84.9 (1)° and 41.5 (1)°, respectively, with the bromo formyl phenyl and methyl phenyl rings. The geometric parameters of the title molecule agrees well with those reported for similar structures (Wang *et al.*, 2011; Hou, 2008).

The molecular structure is stabilized by intramolecular C14—H14···O3 hydrogen bond which generates an S(7) ring motif. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds. The molecules at *x, y, z* and *1-x, -y, -z* are linked by C19—H19B···O1 hydrogen bonds into cyclic centrosymmetric $R_2^2(16)$ dimers. The dimers are linked by the C5—H5···O4 hydrogen bond forming supramolecular tapes running along the [100] directions (Fig. 2). The crystal packing is further stabilized by C—H···π interactions between a methyl H19C atom and a neighbouring benzene ring (C13-C18), with a C19—H19C···Cg^{iii} separation of 2.74 Å (Fig. 3 and Table 1; Cg is the centroid of the C13-C18 benzene ring, Symmetry code as in Fig. 3).

S2. Experimental

A solution of salicylaldehyde (3.7 mmol, 0.74g) and potassium carbonate (5.59 mmol, 0.77g) in acetonitrile as solvent (10ml) was stirred for 15 minutes at room temperature. To this solution, (Z-methyl 2-(bromomethyl)-3-o-tolylacrylate (3.7 mmol, 1g) was added dropwise. After the completion of the reaction as indicated by TLC, acetonitrile was evaporated. Ethylacetate (15ml) and water (15ml) were added to the crude mass and extracted. The organic layer was dried over anhydrous sodium sulfate. Removal of the solvent led to the crude product which was purified through pad of silica gel (100-200 mesh) using ethylacetate and hexanes (1:9) as solvents. The pure title compound was obtained as a colorless solid (1.32g, 91%). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a ethyl-acetate solution at room temperature.

S3. Refinement

All H atoms were positioned geometrically, with C-H = 0.93 - 0.96 Å and constrained to ride on their parent atom, with U_{iso}(H)=1.5U_{eq} for methyl and hydroxyl H atoms and 1.2U_{eq}(C) for other H atoms.

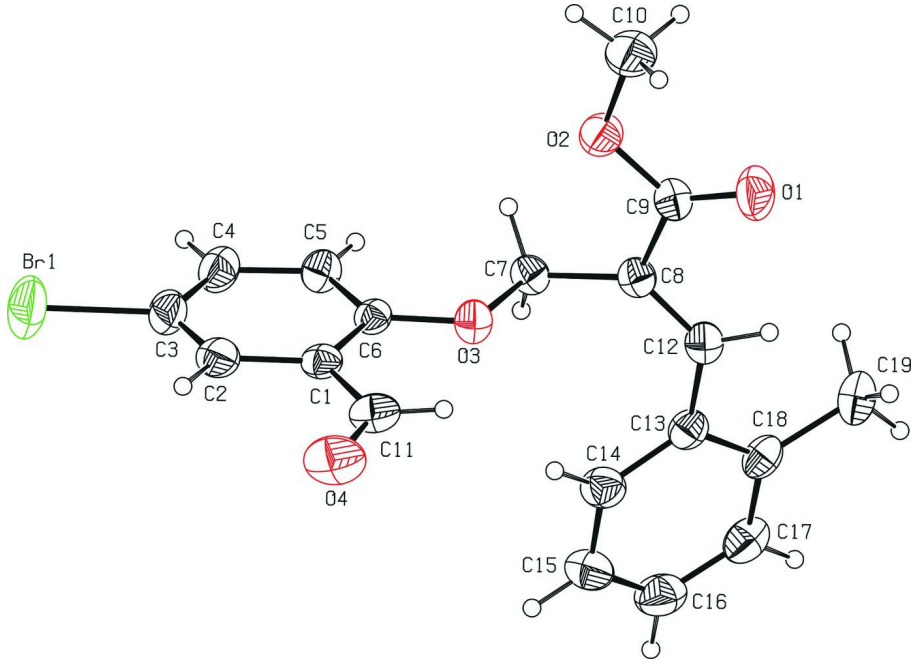

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small cycles of arbitrary radius.

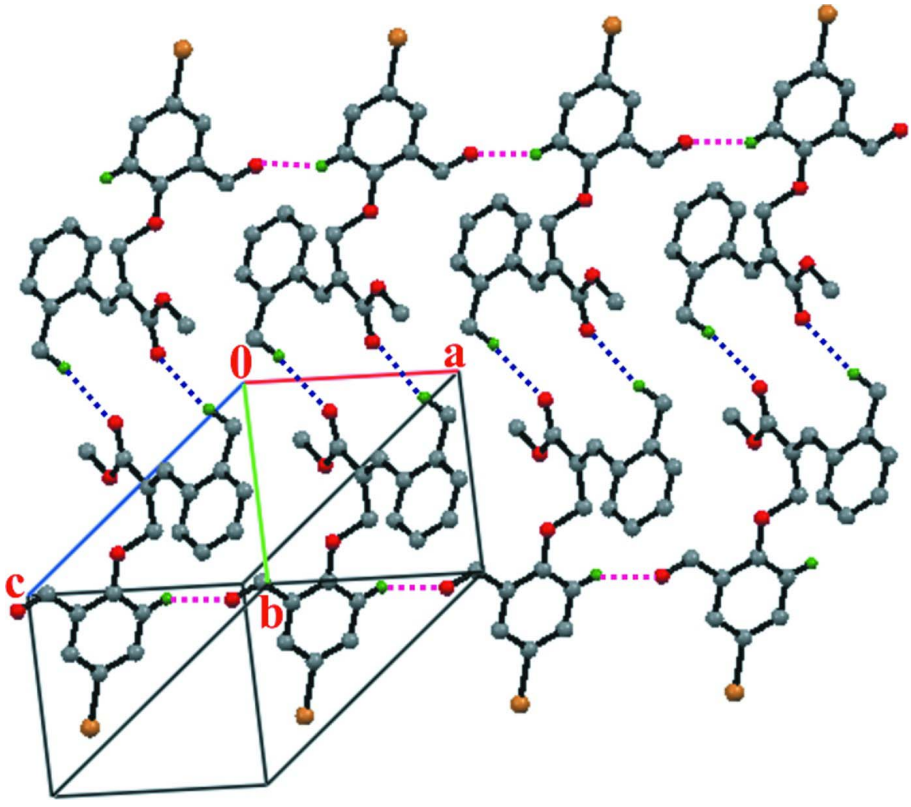

Figure 2

Supramolecular tape formation in the crystal packing of the title compound whereby centrosymmetrc $R_2^2(16)$ dimeric aggregates sustained by C—H···O (blue dashed lines) contacts are linked via C—H···O contacts (magenta dashed lines) along [1 0 0].

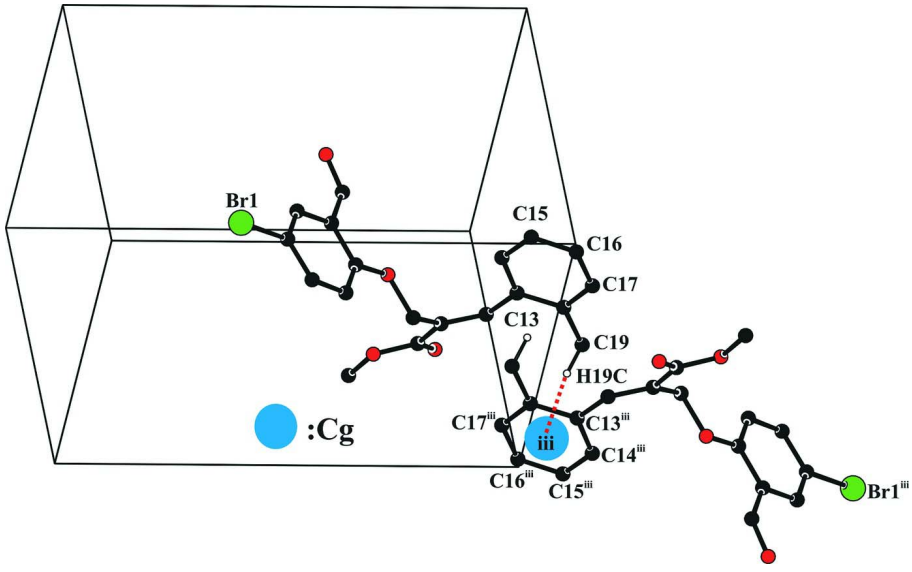

Figure 3

A view of the C-H···π interactions (dotted lines) in the crystal structure of the title compound. Cg denotes centroid of the C13-C18 benzene ring. [Symmetry code: (iii) 2-x, 1-y, -z.]

(*Z*)-Methyl 2-[(4-bromo-2-formylphenoxy)methyl]-3-*o*-tolylacrylate

Crystal data

$C_{19}H_{17}BrO_4$
$M_r = 389.24$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0114$ (2) Å
$b = 8.6138$ (2) Å
$c = 13.4827$ (4) Å
$\alpha = 96.466$ (1)°
$\beta = 97.185$ (1)°
$\gamma = 106.546$ (2)°
$V = 874.08$ (4) Å^3
$Z = 2$
$F(000) = 396$
$D_x = 1.479$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5491 reflections
$\theta = 1.5$–$30.8°$
$\mu = 2.37$ mm^{-1}
$T = 293$ K
Block, colourless
0.25 × 0.23 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.547$, $T_{max} = 0.653$
21788 measured reflections
5440 independent reflections
2870 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 30.8°$, $\theta_{min} = 2.5°$
$h = -11 \rightarrow 8$
$k = -9 \rightarrow 12$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.125$
$S = 1.02$
5440 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
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.2207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ 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.

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 $F^2 > 2$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}
C1	0.5938 (3)	0.6570 (2)	0.44131 (14)	0.0451 (4)
C2	0.6433 (3)	0.7625 (3)	0.53364 (16)	0.0582 (6)
H2	0.5581	0.7944	0.5644	0.070*

C3	0.8167 (4)	0.8193 (3)	0.57901 (16)	0.0628 (6)
C4	0.9439 (3)	0.7725 (3)	0.53421 (17)	0.0620 (6)
H4	1.0614	0.8124	0.5654	0.074*
C5	0.8989 (3)	0.6674 (3)	0.44374 (16)	0.0522 (5)
H5	0.9853	0.6360	0.4140	0.063*
C6	0.7237 (2)	0.6087 (2)	0.39719 (14)	0.0419 (4)
C7	0.7942 (2)	0.4478 (2)	0.26070 (15)	0.0460 (4)
H7A	0.8629	0.4046	0.3086	0.055*
H7B	0.8741	0.5375	0.2364	0.055*
C8	0.6943 (3)	0.3164 (2)	0.17415 (15)	0.0462 (4)
C9	0.6192 (3)	0.1482 (3)	0.19567 (16)	0.0514 (5)
C10	0.5959 (4)	−0.0215 (3)	0.3216 (2)	0.0829 (8)
H10A	0.4703	−0.0646	0.3009	0.124*
H10B	0.6242	−0.0147	0.3936	0.124*
H10C	0.6521	−0.0925	0.2885	0.124*
C11	0.4093 (3)	0.6015 (3)	0.39152 (18)	0.0588 (6)
H11	0.3784	0.5237	0.3333	0.071*
C12	0.6729 (3)	0.3375 (3)	0.07702 (15)	0.0494 (5)
H12	0.6170	0.2431	0.0304	0.059*
C13	0.7263 (2)	0.4903 (3)	0.03471 (15)	0.0490 (5)
C14	0.7153 (3)	0.6369 (3)	0.08434 (18)	0.0598 (5)
H14	0.6751	0.6385	0.1461	0.072*
C15	0.7630 (4)	0.7799 (3)	0.0434 (2)	0.0711 (7)
H15	0.7554	0.8770	0.0775	0.085*
C16	0.8218 (4)	0.7776 (3)	−0.0476 (2)	0.0743 (7)
H16	0.8566	0.8742	−0.0747	0.089*
C17	0.8297 (3)	0.6337 (3)	−0.09913 (18)	0.0651 (6)
H17	0.8673	0.6340	−0.1617	0.078*
C18	0.7828 (3)	0.4878 (3)	−0.06005 (15)	0.0531 (5)
C19	0.7942 (3)	0.3325 (3)	−0.11804 (17)	0.0655 (6)
H19A	0.8274	0.3532	−0.1824	0.098*
H19B	0.6814	0.2499	−0.1283	0.098*
H19C	0.8810	0.2951	−0.0804	0.098*
O1	0.5339 (3)	0.0321 (2)	0.13521 (13)	0.0794 (5)
O2	0.6575 (2)	0.13951 (18)	0.29434 (12)	0.0652 (4)
O3	0.66638 (17)	0.50451 (17)	0.30849 (10)	0.0497 (3)
O4	0.2955 (2)	0.6501 (3)	0.42096 (16)	0.0877 (6)
Br1	0.88459 (5)	0.96282 (4)	0.70416 (2)	0.10598 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0500 (11)	0.0487 (11)	0.0443 (10)	0.0191 (9)	0.0157 (9)	0.0186 (8)
C2	0.0751 (16)	0.0628 (13)	0.0495 (11)	0.0316 (12)	0.0236 (11)	0.0185 (10)
C3	0.0861 (18)	0.0606 (13)	0.0405 (10)	0.0204 (12)	0.0117 (11)	0.0069 (9)
C4	0.0599 (13)	0.0636 (14)	0.0521 (12)	0.0087 (11)	−0.0021 (10)	0.0051 (10)
C5	0.0449 (11)	0.0578 (12)	0.0510 (11)	0.0123 (10)	0.0073 (9)	0.0060 (9)
C6	0.0445 (10)	0.0420 (10)	0.0391 (9)	0.0107 (8)	0.0080 (8)	0.0116 (8)

C7	0.0394 (10)	0.0467 (10)	0.0528 (11)	0.0139 (8)	0.0105 (8)	0.0051 (8)
C8	0.0423 (10)	0.0476 (11)	0.0491 (11)	0.0139 (9)	0.0104 (8)	0.0048 (8)
C9	0.0536 (12)	0.0490 (11)	0.0504 (11)	0.0142 (10)	0.0107 (9)	0.0035 (9)
C10	0.106 (2)	0.0545 (14)	0.0797 (18)	0.0085 (14)	0.0066 (15)	0.0254 (13)
C11	0.0498 (12)	0.0710 (14)	0.0669 (14)	0.0253 (11)	0.0187 (11)	0.0282 (12)
C12	0.0434 (10)	0.0529 (12)	0.0499 (11)	0.0135 (9)	0.0078 (9)	0.0027 (9)
C13	0.0396 (10)	0.0567 (12)	0.0482 (11)	0.0134 (9)	0.0021 (8)	0.0073 (9)
C14	0.0595 (13)	0.0647 (14)	0.0619 (13)	0.0268 (11)	0.0123 (11)	0.0137 (11)
C15	0.0777 (16)	0.0630 (15)	0.0803 (18)	0.0342 (13)	0.0083 (14)	0.0139 (13)
C16	0.0793 (17)	0.0678 (16)	0.0757 (17)	0.0188 (14)	0.0051 (14)	0.0284 (14)
C17	0.0607 (14)	0.0744 (16)	0.0530 (13)	0.0085 (12)	0.0033 (10)	0.0187 (12)
C18	0.0398 (10)	0.0650 (13)	0.0457 (11)	0.0067 (10)	−0.0025 (8)	0.0072 (10)
C19	0.0609 (14)	0.0723 (15)	0.0493 (12)	0.0043 (12)	0.0074 (10)	−0.0049 (11)
O1	0.1097 (14)	0.0511 (9)	0.0574 (9)	0.0001 (9)	0.0075 (9)	−0.0037 (8)
O2	0.0781 (11)	0.0482 (9)	0.0593 (9)	0.0066 (8)	−0.0001 (8)	0.0129 (7)
O3	0.0386 (7)	0.0575 (8)	0.0496 (8)	0.0131 (6)	0.0068 (6)	−0.0009 (6)
O4	0.0632 (11)	0.1185 (16)	0.1058 (15)	0.0513 (11)	0.0325 (10)	0.0350 (12)
Br1	0.1485 (4)	0.1068 (3)	0.05066 (17)	0.0334 (2)	0.00845 (17)	−0.01403 (15)

Geometric parameters (Å, º)

C1—C2	1.396 (3)	C10—H10A	0.9600
C1—C6	1.398 (3)	C10—H10B	0.9600
C1—C11	1.464 (3)	C10—H10C	0.9600
C2—C3	1.370 (3)	C11—O4	1.197 (3)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.378 (3)	C12—C13	1.466 (3)
C3—Br1	1.895 (2)	C12—H12	0.9300
C4—C5	1.376 (3)	C13—C14	1.392 (3)
C4—H4	0.9300	C13—C18	1.408 (3)
C5—C6	1.387 (3)	C14—C15	1.380 (3)
C5—H5	0.9300	C14—H14	0.9300
C6—O3	1.354 (2)	C15—C16	1.369 (4)
C7—O3	1.443 (2)	C15—H15	0.9300
C7—C8	1.496 (3)	C16—C17	1.373 (4)
C7—H7A	0.9700	C16—H16	0.9300
C7—H7B	0.9700	C17—C18	1.389 (3)
C8—C12	1.339 (3)	C17—H17	0.9300
C8—C9	1.478 (3)	C18—C19	1.504 (3)
C9—O1	1.191 (3)	C19—H19A	0.9600
C9—O2	1.343 (3)	C19—H19B	0.9600
C10—O2	1.440 (3)	C19—H19C	0.9600
C2—C1—C6	118.86 (19)	H10A—C10—H10C	109.5
C2—C1—C11	119.93 (19)	H10B—C10—H10C	109.5
C6—C1—C11	121.20 (19)	O4—C11—C1	124.1 (2)
C3—C2—C1	120.2 (2)	O4—C11—H11	117.9
C3—C2—H2	119.9	C1—C11—H11	117.9

C1—C2—H2	119.9	C8—C12—C13	128.39 (19)
C2—C3—C4	120.4 (2)	C8—C12—H12	115.8
C2—C3—Br1	120.44 (18)	C13—C12—H12	115.8
C4—C3—Br1	119.17 (19)	C14—C13—C18	119.1 (2)
C5—C4—C3	120.6 (2)	C14—C13—C12	121.34 (19)
C5—C4—H4	119.7	C18—C13—C12	119.46 (19)
C3—C4—H4	119.7	C15—C14—C13	121.1 (2)
C4—C5—C6	119.5 (2)	C15—C14—H14	119.4
C4—C5—H5	120.2	C13—C14—H14	119.4
C6—C5—H5	120.2	C16—C15—C14	119.5 (2)
O3—C6—C5	123.87 (17)	C16—C15—H15	120.2
O3—C6—C1	115.80 (17)	C14—C15—H15	120.2
C5—C6—C1	120.33 (18)	C15—C16—C17	120.4 (2)
O3—C7—C8	107.34 (15)	C15—C16—H16	119.8
O3—C7—H7A	110.2	C17—C16—H16	119.8
C8—C7—H7A	110.2	C16—C17—C18	121.5 (2)
O3—C7—H7B	110.2	C16—C17—H17	119.2
C8—C7—H7B	110.2	C18—C17—H17	119.2
H7A—C7—H7B	108.5	C17—C18—C13	118.2 (2)
C12—C8—C9	116.79 (19)	C17—C18—C19	120.2 (2)
C12—C8—C7	124.91 (19)	C13—C18—C19	121.5 (2)
C9—C8—C7	118.25 (18)	C18—C19—H19A	109.5
O1—C9—O2	122.5 (2)	C18—C19—H19B	109.5
O1—C9—C8	125.9 (2)	H19A—C19—H19B	109.5
O2—C9—C8	111.64 (18)	C18—C19—H19C	109.5
O2—C10—H10A	109.5	H19A—C19—H19C	109.5
O2—C10—H10B	109.5	H19B—C19—H19C	109.5
H10A—C10—H10B	109.5	C9—O2—C10	115.46 (19)
O2—C10—H10C	109.5	C6—O3—C7	118.17 (15)

C6—C1—C2—C3	1.0 (3)	C9—C8—C12—C13	177.09 (19)
C11—C1—C2—C3	−177.82 (19)	C7—C8—C12—C13	−5.6 (3)
C1—C2—C3—C4	−0.2 (3)	C8—C12—C13—C14	−37.2 (3)
C1—C2—C3—Br1	179.89 (15)	C8—C12—C13—C18	145.6 (2)
C2—C3—C4—C5	−0.5 (4)	C18—C13—C14—C15	−1.7 (3)
Br1—C3—C4—C5	179.47 (17)	C12—C13—C14—C15	−179.0 (2)
C3—C4—C5—C6	0.3 (3)	C13—C14—C15—C16	0.2 (4)
C4—C5—C6—O3	−179.72 (19)	C14—C15—C16—C17	1.4 (4)
C4—C5—C6—C1	0.5 (3)	C15—C16—C17—C18	−1.5 (4)
C2—C1—C6—O3	179.09 (17)	C16—C17—C18—C13	0.0 (3)
C11—C1—C6—O3	−2.1 (3)	C16—C17—C18—C19	−179.6 (2)
C2—C1—C6—C5	−1.2 (3)	C14—C13—C18—C17	1.5 (3)
C11—C1—C6—C5	177.62 (19)	C12—C13—C18—C17	178.89 (19)
O3—C7—C8—C12	100.2 (2)	C14—C13—C18—C19	−178.89 (19)
O3—C7—C8—C9	−82.5 (2)	C12—C13—C18—C19	−1.5 (3)
C12—C8—C9—O1	−4.1 (3)	O1—C9—O2—C10	2.9 (3)
C7—C8—C9—O1	178.4 (2)	C8—C9—O2—C10	−177.5 (2)
C12—C8—C9—O2	176.27 (18)	C5—C6—O3—C7	1.6 (3)

C7—C8—C9—O2	−1.2 (3)	C1—C6—O3—C7	−178.66 (16)
C2—C1—C11—O4	5.7 (3)	C8—C7—O3—C6	171.39 (15)
C6—C1—C11—O4	−173.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O3	0.93	2.59	3.377 (3)	143
C19—H19*B*···O1^{i}	0.96	2.53	3.436 (3)	157
C5—H5···O4^{ii}	0.93	2.44	3.273 (3)	149
C19—H19*C*···*Cg*^{iii}	0.96	2.74	3.580 (3)	147

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