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14-Bromo-12-chloro-2,16-dioxapentacyclo[7.7.5.0^{1,21}.0^{3,8}.0^{10,15}]henicosa-3(8),10,12,14-tetraene-7,20-dione

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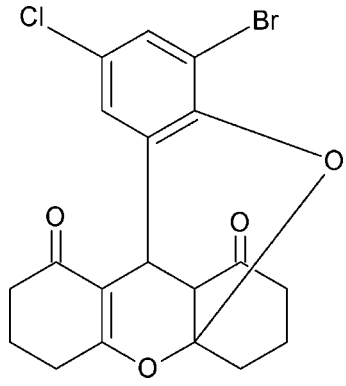
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.007 Å; R factor = 0.058; wR factor = 0.134; data-to-parameter ratio = 15.6.

In the title compound, $C_{19}H_{16}BrClO_4$, both the fused xanthene rings and one of the cyclohexane rings adopt envelope conformations, while the other cyclohexane ring is in a chair conformation. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming infinite chains running along [10$\bar{1}$] incorporating $R_2^2(16)$ ring motifs. In addition, C—H···π interactions and weak π–π stacking interactions [centroid–centroid distance = 3.768 (3) Å] help to consolidate the packing.

Related literature

For similar structures, see: Mohamed *et al.* (2012*b*); Lu *et al.* (2011); Abdelhamid *et al.* (2011). For the bioactiviy of xanthenones, see: Mohamed *et al.* (2012*a*); Gobbi *et al.* (2006); Na (2009). For ring conformations, see: Cremer and Pople (1975).



Experimental

Crystal data

$C_{19}H_{16}BrClO_4$
M_r = 423.67
Monoclinic, $P2_1/n$
a = 10.2741 (6) Å
b = 10.2800 (6) Å
c = 15.8581 (8) Å
β = 102.073 (5)°
V = 1637.85 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.70 mm^{-1}
T = 123 K
0.25 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.529, T_{max} = 0.616
7243 measured reflections
3516 independent reflections
2547 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.134
S = 1.04
3516 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

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

*Cg*3 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···O3^{i}	0.99	2.53	3.407 (6)	147
C9—H9B···Cg3^{ii}	0.99	2.89	3.731 (5)	143

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

This work was supported financially by the Higher Education Ministry of Egypt. The authors gratefully acknowledge Manchester Metropolitan University, the University of Strathclyde and Erciyes University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7072).

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supplementary materials

Acta Cryst. (2013). E**69**, o769–o770 [doi:10.1107/S1600536813010374]

14-Bromo-12-chloro-2,16-dioxapentacyclo-[7.7.5.$0^{1,21}$.$0^{3,8}$.$0^{10,15}$]henicosa-3(8),10,12,14-tetraene-7,20-dione

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Comment

Xanthenones have very diverse biological profiles, including antihypertensive, anti-oxidative, antithrombotic and anticancer activity, depending on their diverse structures, which are modified by substituents on the ring system (Gobbi *et al.*, 2006; Na, 2009). Following to our earlier study on synthesis of series of the bioactive oxanthenediones (Abdelhamid *et al.*, 2011), acridinediones (Mohamed *et al.*, 2012*a*) and benzopyranes (Mohamed *et al.*, 2012*b*) we became interested in synthesizing the title compound to investigate the relationship between antibacterial activity and structure.

In the title compound, (Fig. 1), the two fused xanthene rings (O2/C7/C12–C14/C19 and O4/C5–C7/C12/C13) adopt envelope conformations [the puckering parameters (Cremer & Pople, 1975) are Q_T = 0.522 (5) Å, θ = 127.4 (5) °, φ = 299.1 (6) ° and Q_T = 0.539 (5) Å, θ = 125.9 (5) °, φ = 51.2 (6) °, respectively], one (C14–C19) of the cyclohexane rings is also in an envelope conformation with puckering parameters of Q_T = 0.440 (5) Å, θ = 129.9 (7) °, φ = 344.4 (9) °, and the other (C7–C12) is in a chair conformation with puckering parameters of Q_T = 0.518 (5) Å, θ = 8.0 (6) °, φ = 84 (4). All the bond lengths and bond angles of the title compound are within the expected values and are comparable with those reported for similar structures (Mohamed *et al.*, 2012*b*; Lu *et al.*, 2011; Abdelhamid *et al.*, 2011).

In the crystal structure, long-range C—H···O hydrogen bonds (Table 1, Fig. 2) connect the adjacent molecules into infinite chains running along [$10\bar{1}$] with $R^2_2(16)$ ring motifs. C–H···π interactions and weak π-π stacking interactions [*Cg*3···*Cg*3^{i}= 3.768 (3) Å; *Cg*3 is a centroid of the C1–C6 benzene ring and symmetry code: (i) = 1 - *x*, 1 - *y*, 1 - *z*] also contribute to the consolidation of the crystal packing.

Experimental

A mixture of 1 mmol (236 mg) 3-bromo-5-chloro-2-hydroxybenzaldehyde, 1 mmol (112 mg) cyclohexane-1,3-dione and 1 mmol (123 mg) (4-aminophenyl)methanol in 50 ml e thanol was refluxed at 350 K. The reaction progress was monitored by TLC till completion after 5 h. Excess solvent was evaporated under vacuum and the resulted solid was filtered, washed with cold ethanol and recrystallized from ethanol to afford 61% of the title compound. Colourless blocks were obtained by slow evaporation of ethanol solution of (I) at room temperature for two days. M.P. 504 K.

Refinement

H atoms bound to C atoms were placed at calculated positions [0.95 (aromatic CH), 0.99 (methylene CH_2) and 1.00 Å (methine CH)] and refined in riding modes with U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

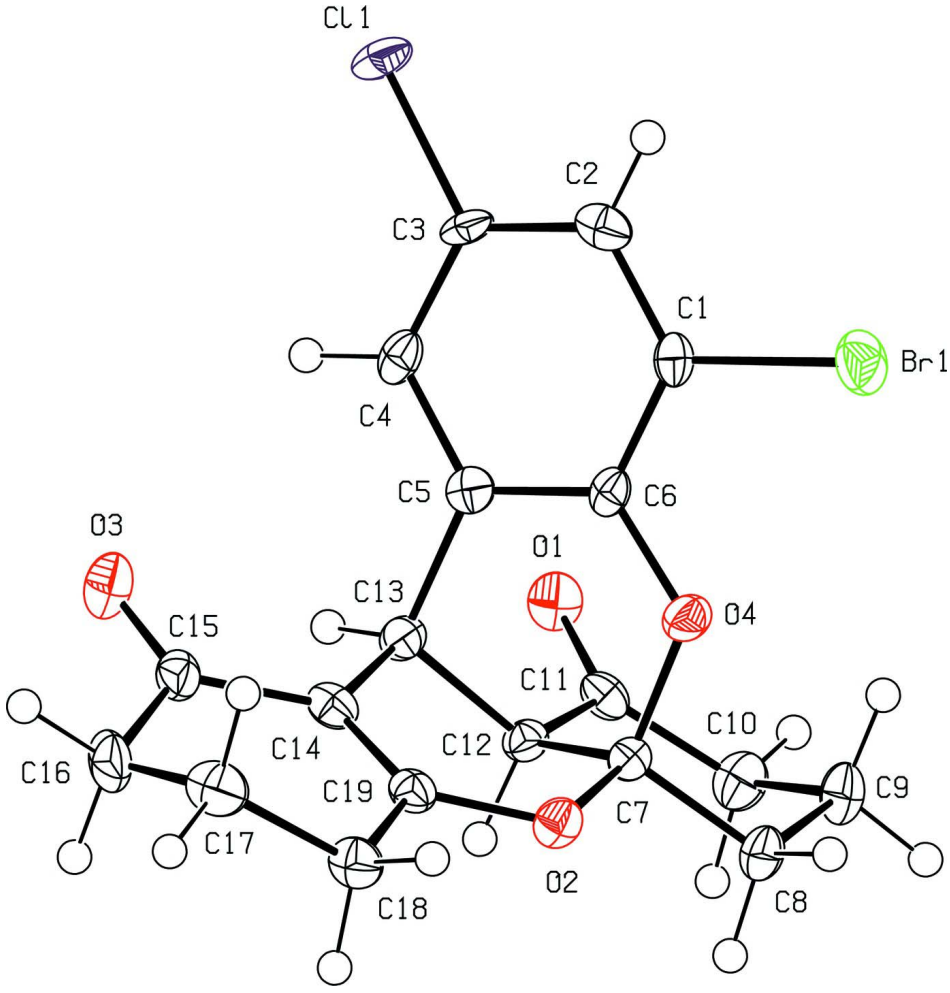

Figure 1

The title compound with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

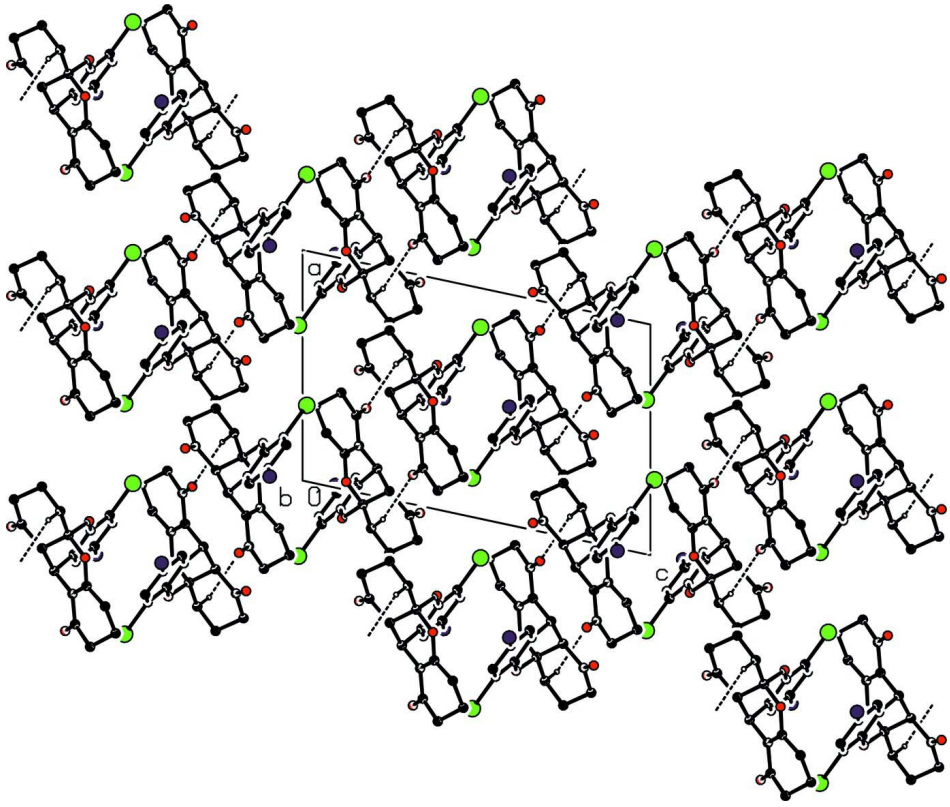

Figure 2

View of the packing and hydrogen bonding diagram of the title compound along the *b* axis.

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Crystal data

$C_{19}H_{16}BrClO_4$
M_r = 423.67
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.2741 (6) Å
b = 10.2800 (6) Å
c = 15.8581 (8) Å
β = 102.073 (5)°
V = 1637.85 (16) Å^3
Z = 4
$F(000)$ = 856
D_x = 1.718 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2011 reflections
θ = 3.0–28.8°
μ = 2.70 mm^{-1}
T = 123 K
Block, colourless
0.25 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0727 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.529, T_{max} = 0.616
7243 measured reflections
3516 independent reflections
2547 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.0°, θ_{min} = 3.3°
h = −13→13
k = −11→12
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.134$
$S = 1.04$
3516 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 3.8105P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.83070 (5)	0.65176 (6)	0.51190 (3)	0.0317 (2)
Cl1	0.48771 (12)	0.24296 (11)	0.40547 (8)	0.0239 (4)
O1	0.5310 (3)	0.6514 (3)	0.1626 (2)	0.0248 (11)
O2	0.4643 (3)	0.9536 (3)	0.37446 (19)	0.0204 (10)
O3	0.1281 (3)	0.6340 (4)	0.3173 (2)	0.0309 (12)
O4	0.6260 (3)	0.7948 (3)	0.3862 (2)	0.0222 (10)
C1	0.6710 (4)	0.5856 (5)	0.4453 (3)	0.0192 (14)
C2	0.6398 (5)	0.4564 (5)	0.4527 (3)	0.0209 (16)
C3	0.5230 (5)	0.4094 (4)	0.4018 (3)	0.0180 (14)
C4	0.4377 (5)	0.4900 (5)	0.3470 (3)	0.0199 (16)
C5	0.4683 (5)	0.6205 (4)	0.3418 (3)	0.0174 (14)
C6	0.5875 (4)	0.6689 (4)	0.3903 (3)	0.0165 (14)
C7	0.5465 (4)	0.8852 (5)	0.3268 (3)	0.0186 (14)
C8	0.6430 (5)	0.9822 (5)	0.3029 (3)	0.0224 (16)
C9	0.7320 (5)	0.9167 (5)	0.2502 (3)	0.0258 (17)
C10	0.6512 (5)	0.8501 (5)	0.1700 (3)	0.0273 (17)
C11	0.5501 (5)	0.7597 (5)	0.1918 (3)	0.0188 (14)
C12	0.4649 (4)	0.8147 (4)	0.2507 (3)	0.0173 (12)
C13	0.3782 (4)	0.7170 (5)	0.2854 (3)	0.0189 (14)
C14	0.2961 (4)	0.7914 (5)	0.3381 (3)	0.0185 (14)
C15	0.1663 (5)	0.7408 (5)	0.3456 (3)	0.0218 (14)
C16	0.0825 (5)	0.8278 (5)	0.3889 (3)	0.0297 (17)
C17	0.1648 (5)	0.9056 (5)	0.4622 (3)	0.0293 (17)
C18	0.2719 (5)	0.9826 (5)	0.4319 (3)	0.0226 (16)
C19	0.3432 (5)	0.9016 (5)	0.3786 (3)	0.0185 (14)
H2	0.69700	0.40090	0.49180	0.0250*

H4	0.35780	0.45610	0.31280	0.0240*
H8A	0.69840	1.01970	0.35590	0.0270*
H8B	0.59310	1.05390	0.26900	0.0270*
H9A	0.78860	0.85130	0.28640	0.0310*
H9B	0.79120	0.98260	0.23250	0.0310*
H10A	0.60600	0.91700	0.12930	0.0320*
H10B	0.71220	0.80100	0.14090	0.0320*
H12	0.40380	0.88020	0.21640	0.0210*
H13	0.31860	0.67080	0.23660	0.0220*
H16A	0.01760	0.77390	0.41160	0.0360*
H16B	0.03170	0.88840	0.34570	0.0360*
H17A	0.10610	0.96580	0.48570	0.0350*
H17B	0.20660	0.84580	0.50900	0.0350*
H18A	0.23100	1.05820	0.39760	0.0270*
H18B	0.33640	1.01600	0.48260	0.0270*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0228 (3)	0.0413 (4)	0.0276 (3)	−0.0031 (2)	−0.0026 (2)	0.0050 (3)
Cl1	0.0344 (7)	0.0103 (6)	0.0300 (6)	−0.0019 (5)	0.0134 (5)	−0.0010 (5)
O1	0.0262 (19)	0.026 (2)	0.0228 (17)	−0.0010 (16)	0.0067 (14)	−0.0059 (16)
O2	0.0222 (18)	0.0182 (18)	0.0219 (17)	−0.0016 (14)	0.0075 (14)	−0.0044 (14)
O3	0.024 (2)	0.034 (2)	0.036 (2)	−0.0078 (17)	0.0092 (16)	−0.0022 (18)
O4	0.0228 (18)	0.0182 (18)	0.0230 (17)	−0.0041 (14)	−0.0012 (14)	0.0016 (14)
C1	0.014 (2)	0.025 (3)	0.020 (2)	−0.002 (2)	0.0066 (19)	−0.001 (2)
C2	0.024 (3)	0.024 (3)	0.018 (2)	0.009 (2)	0.012 (2)	0.004 (2)
C3	0.026 (3)	0.008 (2)	0.023 (2)	0.0001 (19)	0.012 (2)	0.0006 (19)
C4	0.020 (3)	0.020 (3)	0.023 (2)	−0.005 (2)	0.012 (2)	−0.005 (2)
C5	0.020 (2)	0.019 (3)	0.016 (2)	0.0013 (19)	0.0102 (19)	−0.0002 (19)
C6	0.016 (2)	0.018 (3)	0.018 (2)	−0.0022 (19)	0.0096 (18)	−0.003 (2)
C7	0.017 (2)	0.016 (3)	0.023 (2)	−0.0007 (19)	0.005 (2)	0.001 (2)
C8	0.020 (3)	0.022 (3)	0.024 (2)	−0.006 (2)	0.002 (2)	−0.004 (2)
C9	0.019 (3)	0.031 (3)	0.029 (3)	−0.005 (2)	0.009 (2)	−0.002 (2)
C10	0.028 (3)	0.028 (3)	0.026 (3)	−0.004 (2)	0.006 (2)	−0.002 (2)
C11	0.018 (2)	0.023 (3)	0.014 (2)	0.004 (2)	0.0001 (18)	0.000 (2)
C12	0.019 (2)	0.016 (2)	0.017 (2)	−0.0011 (19)	0.0037 (18)	0.0021 (19)
C13	0.020 (2)	0.017 (3)	0.019 (2)	−0.002 (2)	0.0026 (19)	0.0011 (19)
C14	0.020 (2)	0.023 (3)	0.013 (2)	0.005 (2)	0.0043 (18)	0.003 (2)
C15	0.017 (2)	0.027 (3)	0.020 (2)	−0.002 (2)	0.0009 (19)	0.007 (2)
C16	0.015 (3)	0.039 (3)	0.037 (3)	0.000 (2)	0.010 (2)	0.008 (3)
C17	0.031 (3)	0.032 (3)	0.028 (3)	0.007 (2)	0.013 (2)	0.006 (2)
C18	0.024 (3)	0.024 (3)	0.022 (2)	0.004 (2)	0.010 (2)	0.000 (2)
C19	0.018 (2)	0.021 (3)	0.017 (2)	0.003 (2)	0.0045 (19)	0.005 (2)

Geometric parameters (Å, º)

Br1—C1	1.883 (5)	C14—C15	1.459 (7)
Cl1—C3	1.753 (4)	C14—C19	1.342 (7)
O1—C11	1.206 (6)	C15—C16	1.503 (7)

O2—C7	1.430 (6)	C16—C17	1.515 (7)
O2—C19	1.368 (6)	C17—C18	1.513 (7)
O3—C15	1.220 (6)	C18—C19	1.484 (7)
O4—C6	1.359 (5)	C2—H2	0.9500
O4—C7	1.448 (6)	C4—H4	0.9500
C1—C2	1.377 (7)	C8—H8A	0.9900
C1—C6	1.385 (6)	C8—H8B	0.9900
C2—C3	1.386 (7)	C9—H9A	0.9900
C3—C4	1.375 (7)	C9—H9B	0.9900
C4—C5	1.384 (7)	C10—H10A	0.9900
C5—C6	1.395 (7)	C10—H10B	0.9900
C5—C13	1.515 (7)	C12—H12	1.0000
C7—C8	1.509 (7)	C13—H13	1.0000
C7—C12	1.504 (6)	C16—H16A	0.9900
C8—C9	1.519 (7)	C16—H16B	0.9900
C9—C10	1.528 (7)	C17—H17A	0.9900
C10—C11	1.487 (7)	C17—H17B	0.9900
C11—C12	1.517 (7)	C18—H18A	0.9900
C12—C13	1.520 (6)	C18—H18B	0.9900
C13—C14	1.513 (7)		

C7—O2—C19	118.5 (4)	O2—C19—C14	123.2 (4)
C6—O4—C7	120.8 (3)	O2—C19—C18	111.7 (4)
Br1—C1—C2	119.5 (4)	C14—C19—C18	125.1 (5)
Br1—C1—C6	118.8 (4)	C1—C2—H2	121.00
C2—C1—C6	121.7 (4)	C3—C2—H2	121.00
C1—C2—C3	118.4 (4)	C3—C4—H4	120.00
Cl1—C3—C2	118.8 (4)	C5—C4—H4	120.00
Cl1—C3—C4	120.0 (4)	C7—C8—H8A	110.00
C2—C3—C4	121.2 (4)	C7—C8—H8B	110.00
C3—C4—C5	119.9 (5)	C9—C8—H8A	110.00
C4—C5—C6	119.8 (4)	C9—C8—H8B	110.00
C4—C5—C13	123.5 (4)	H8A—C8—H8B	108.00
C6—C5—C13	116.7 (4)	C8—C9—H9A	109.00
O4—C6—C1	118.1 (4)	C8—C9—H9B	109.00
O4—C6—C5	123.0 (4)	C10—C9—H9A	109.00
C1—C6—C5	118.9 (4)	C10—C9—H9B	109.00
O2—C7—O4	106.7 (3)	H9A—C9—H9B	108.00
O2—C7—C8	107.4 (4)	C9—C10—H10A	109.00
O2—C7—C12	111.7 (3)	C9—C10—H10B	109.00
O4—C7—C8	106.1 (3)	C11—C10—H10A	109.00
O4—C7—C12	110.9 (4)	C11—C10—H10B	109.00
C8—C7—C12	113.7 (4)	H10A—C10—H10B	108.00
C7—C8—C9	110.4 (4)	C7—C12—H12	107.00
C8—C9—C10	111.8 (4)	C11—C12—H12	107.00
C9—C10—C11	111.8 (4)	C13—C12—H12	107.00
O1—C11—C10	123.6 (5)	C5—C13—H13	110.00
O1—C11—C12	120.8 (4)	C12—C13—H13	110.00
C10—C11—C12	115.6 (4)	C14—C13—H13	110.00

C7—C12—C11	112.2 (4)	C15—C16—H16A	109.00
C7—C12—C13	107.4 (4)	C15—C16—H16B	109.00
C11—C12—C13	115.7 (4)	C17—C16—H16A	109.00
C5—C13—C12	108.3 (4)	C17—C16—H16B	109.00
C5—C13—C14	110.3 (4)	H16A—C16—H16B	108.00
C12—C13—C14	107.6 (4)	C16—C17—H17A	109.00
C13—C14—C15	119.3 (4)	C16—C17—H17B	109.00
C13—C14—C19	120.3 (4)	C18—C17—H17A	109.00
C15—C14—C19	120.4 (4)	C18—C17—H17B	109.00
O3—C15—C14	121.3 (5)	H17A—C17—H17B	108.00
O3—C15—C16	122.2 (5)	C17—C18—H18A	109.00
C14—C15—C16	116.5 (4)	C17—C18—H18B	109.00
C15—C16—C17	112.6 (4)	C19—C18—H18A	109.00
C16—C17—C18	111.0 (4)	C19—C18—H18B	109.00
C17—C18—C19	111.5 (4)	H18A—C18—H18B	108.00

C19—O2—C7—O4	−88.4 (4)	O4—C7—C12—C11	−70.2 (5)
C19—O2—C7—C8	158.3 (4)	O4—C7—C12—C13	58.0 (4)
C19—O2—C7—C12	32.9 (5)	C8—C7—C12—C11	49.2 (5)
C7—O2—C19—C14	−2.0 (7)	C8—C7—C12—C13	177.4 (4)
C7—O2—C19—C18	178.7 (4)	C7—C8—C9—C10	55.9 (5)
C7—O4—C6—C1	176.9 (4)	C8—C9—C10—C11	−53.0 (6)
C7—O4—C6—C5	−3.2 (6)	C9—C10—C11—O1	−134.8 (5)
C6—O4—C7—O2	96.0 (4)	C9—C10—C11—C12	48.4 (6)
C6—O4—C7—C8	−149.7 (4)	O1—C11—C12—C7	136.7 (5)
C6—O4—C7—C12	−25.8 (5)	O1—C11—C12—C13	13.0 (6)
Br1—C1—C2—C3	−178.8 (4)	C10—C11—C12—C7	−46.4 (5)
C6—C1—C2—C3	1.6 (7)	C10—C11—C12—C13	−170.0 (4)
Br1—C1—C6—O4	0.9 (6)	C7—C12—C13—C5	−62.3 (5)
Br1—C1—C6—C5	−179.1 (3)	C7—C12—C13—C14	57.0 (4)
C2—C1—C6—O4	−179.5 (4)	C11—C12—C13—C5	63.8 (5)
C2—C1—C6—C5	0.5 (7)	C11—C12—C13—C14	−176.9 (4)
C1—C2—C3—Cl1	175.9 (4)	C5—C13—C14—C15	−90.3 (5)
C1—C2—C3—C4	−2.0 (7)	C5—C13—C14—C19	88.6 (6)
Cl1—C3—C4—C5	−177.6 (4)	C12—C13—C14—C15	151.7 (4)
C2—C3—C4—C5	0.3 (8)	C12—C13—C14—C19	−29.4 (6)
C3—C4—C5—C6	1.9 (7)	C13—C14—C15—O3	7.1 (7)
C3—C4—C5—C13	−178.0 (4)	C13—C14—C15—C16	−172.2 (4)
C4—C5—C6—O4	177.7 (4)	C19—C14—C15—O3	−171.9 (5)
C4—C5—C6—C1	−2.3 (7)	C19—C14—C15—C16	8.8 (7)
C13—C5—C6—O4	−2.4 (7)	C13—C14—C19—O2	0.7 (7)
C13—C5—C6—C1	177.6 (4)	C13—C14—C19—C18	180.0 (4)
C4—C5—C13—C12	−144.7 (5)	C15—C14—C19—O2	179.7 (4)
C4—C5—C13—C14	97.8 (5)	C15—C14—C19—C18	−1.1 (8)
C6—C5—C13—C12	35.4 (6)	O3—C15—C16—C17	144.8 (5)
C6—C5—C13—C14	−82.2 (5)	C14—C15—C16—C17	−35.9 (6)
O2—C7—C8—C9	−178.8 (4)	C15—C16—C17—C18	54.9 (6)
O4—C7—C8—C9	67.5 (5)	C16—C17—C18—C19	−46.2 (6)
C12—C7—C8—C9	−54.7 (5)	C17—C18—C19—O2	−160.1 (4)

O2—C7—C12—C11	171.0 (4)	C17—C18—C19—C14	20.5 (7)
O2—C7—C12—C13	−60.8 (5)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···O3^{i}	0.99	2.53	3.407 (6)	147
C9—H9*B*···*Cg*3^{ii}	0.99	2.89	3.731 (5)	143

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2.