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trans,trans,trans-2,3,5,8-Tetrabromo-1,4-dihydroxy-1,2,3,4-tetrahydronaphthalene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.082
Data-to-parameter ratio = 21.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

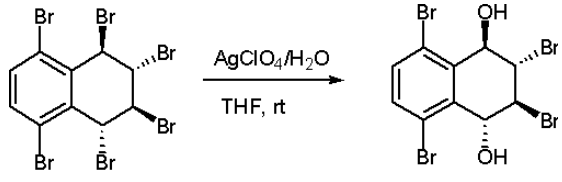
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The structure of the title compound, $C_{10}H_8Br_4O_2$, has been determined at room temperature. The ten-membered tetrahydronaphthalene ring system is nearly planar, with a total puckering amplitude Q_T of 0.386 (5) Å. The crystal structure is stabilized by short inter- and intramolecular hydrogen-bond contacts.

Comment

Naphthalenes, playing an important role as structural units or key intermediates of naturally occurring alkaloids, attract the interest of synthetic and natural product chemists for their biological activities (Huang & Wang, 2001). Halogenated aromatic compounds are an important class of molecules in synthetic organic chemistry. They are key intermediates in the preparation of organometallic reagents (Wakefield, 1976; Davis, 1982; Cannon & Krow, 1996) and play vital roles in transition-metal-mediated coupling reactions (Still, 1985; Miyaura & Suzuki, 1995; Beletskaya & Cheprakov, 2000; Cabri & Candiani, 1995; Meijere & Meyer, 1994; Sonogashira, 1991). Numerous industrially valuable products such as pesticides, insecticides, herbicides, pharmaceutically and medicinally active compounds, fire retardants, and other new materials carry halogen functionality. Hydroxy derivatives of naphthalene have importance for natural products (Kawazoe *et al.*, 1999), as well as for their pharmacological properties (Orsini *et al.*, 2002), and they are useful precursors of other valuable naphthalene derivatives (Ogata *et al.*, 2004). In this study, the crystal structure of the title compound, (II), was determined by X-ray analysis and the molecular structure and the numbering scheme are shown in Fig. 1. Selected geometric parameters are given in Table 1 and their values are normal.



(I) (II)

The geometry of (II) compares well with similar structures reported in the literature (Allen *et al.*, 1987). The mean O—C and Br—C bond distances are 1.422 (6) and 1.938 (5) Å, respectively, with Br—C—C bond angles in the range 107.0 (3)–121.6 (4)° [average values for related compounds: 112.6 (7) (Hökelek *et al.*, 2001), 113.9 (7) (Hökelek *et al.*, 1998) and 115.1 (6)° (Hökelek *et al.*, 1991)]. The ten-membered tetrahydronaphthalene ring system of (II) has the

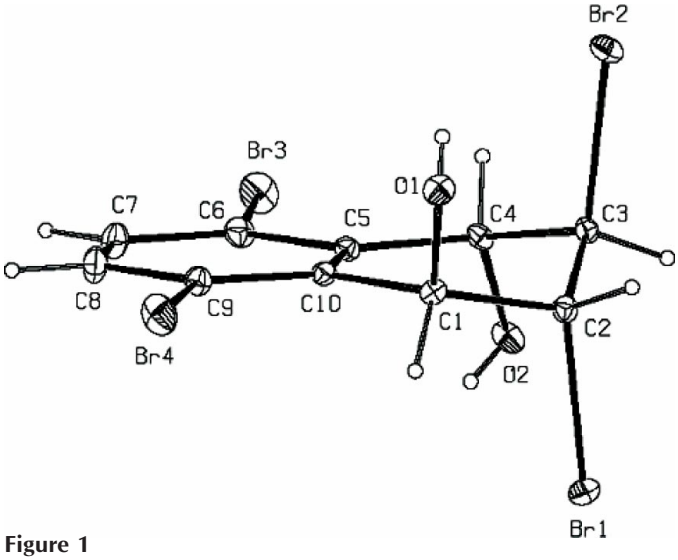


Figure 1
A view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 10% probability level and H atoms are shown as small spheres of arbitrary radii.

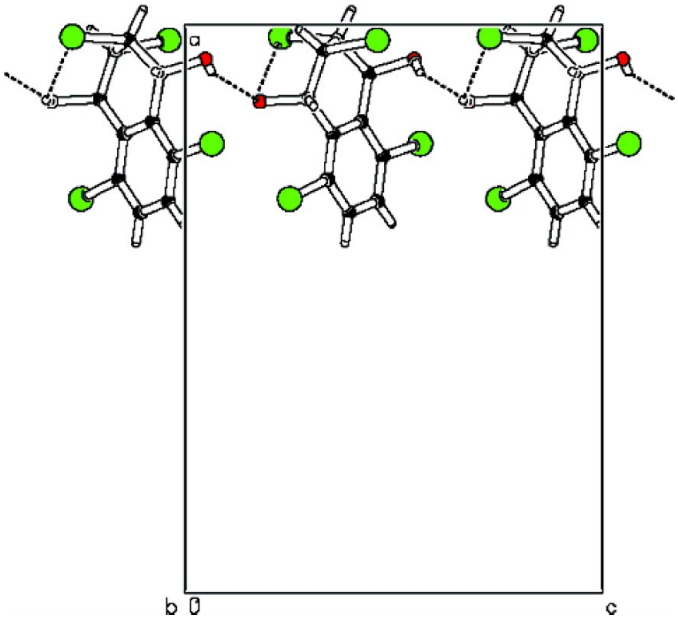


Figure 2
A view of part of the molecular packing and hydrogen bonding in the unit cell of (II).

hydroxy O, Br and H atoms in a *trans,trans,trans* configuration. The maximum deviations from the mean plane of the ring system are −0.058 (5), 0.263 (5) and −0.255 (5) Å for atoms C1, C2 and C3, respectively. The total puckering amplitude Q_T is 0.386 (5) Å (Cremer & Pople, 1975). The crystal structure is stabilized by inter- and intramolecular hydrogen-bonding contacts, involving both hydroxy groups, leading to the formation of chains along the *c* axis (Fig. 2 and Table 2).

Experimental

(1*R*,2*S*,3*S*,4*R*)-1,2,3,4,5,8-Hexabromo-1,2,3,4-tetrahydronaphthalene, (I), was treated with a solution of $AgCl_4{\cdot}nH_2O$ (2.45 g, 10.9 mmol) in aqueous THF (7 ml THF/3 ml H_4O) (Erenler & Çakmak, 2004) to form the title diol (II) (m.p. 461–462 K). This was isolated by column chromatography and purified by crystallization from acetone–hexane.

Crystal data

$C_{10}H_8Br_4O_2$
M_r = 479.76
Orthorhombic, *Pbca*
a = 16.8495 (9) Å
b = 12.1086 (9) Å
c = 12.3570 (7) Å
V = 2521.1 (3) Å^3
Z = 8
D_x = 2.528 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3257 reflections
θ = 1.7–28.9°
μ = 12.75 mm^{-1}
T = 293 K
Plate, colorless
0.64 × 0.41 × 0.12 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.045, T_{max} = 0.310
15995 measured reflections
3257 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 28.8°
h = −22 → 22
k = −16 → 15
l = −13 → 16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.082
S = 1.02
3257 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0198P)^2 + 5.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C2	1.978 (5)	Br4—C9	1.897 (5)
Br2—C3	1.982 (5)	O1—C1	1.429 (6)
Br3—C6	1.895 (5)	O2—C4	1.415 (6)
O1—C1—C2	109.4 (4)	O2—C4—C5	112.5 (4)
O1—C1—C10	111.8 (4)	O2—C4—C3	108.6 (4)
Br1—C2—C1	108.1 (3)	Br3—C6—C5	121.4 (4)
Br1—C2—C3	107.0 (3)	Br3—C6—C7	116.2 (4)
Br2—C3—C4	108.3 (3)	Br4—C9—C10	121.6 (4)
Br2—C3—C2	107.0 (3)	Br4—C9—C8	116.4 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—HO1···Br2	0.62 (7)	2.81 (9)	3.232 (5)	130 (10)
O2—HO2···O1^{i}	0.64 (6)	2.25 (6)	2.840 (6)	155 (7)

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

The hydroxyl H atoms were found in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically, with C—H distances of 0.93 Å for aromatic and 0.98 Å for methylene H atoms, and allowed to ride with, U_{iso}(H) = 1.2U_{eq}(carrier atom).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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trans,trans,trans-2,3,5,8-Tetrabromo-1,4-dihydroxy-1,2,3,4-tetrahydronaphthalene

Mehmet Akkurt, İsmail Çelik, Ramazan Erenler, Osman Çakmak, Cem Cüneyt Ersanlı and Orhan Büyükgüngör

***trans,trans,trans*-2,3,5,8-Tetrabromo-1,4-dihydroxy-1,2,3,4- tetrahydronaphthalene**

Crystal data

$C_{10}H_8Br_4O_2$
$M_r = 479.76$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 16.8495$ (9) Å
$b = 12.1086$ (9) Å
$c = 12.3570$ (7) Å
$V = 2521.1$ (3) Å^3
$Z = 8$
$F(000) = 1792$
$D_x = 2.528$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3257 reflections
$\theta = 1.7$–$28.9°$
$\mu = 12.75$ mm^{-1}
$T = 293$ K
Plate, colorless
0.64 × 0.41 × 0.12 mm

Data collection

Stoe IPDS-II diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.045$, $T_{max} = 0.310$
15995 measured reflections
3257 independent reflections
2283 reflections with $I > 2\sigma(I)$
$R_{int} = 0.089$
$\theta_{max} = 28.8°$, $\theta_{min} = 2.4°$
$h = -22 \rightarrow 22$
$k = -16 \rightarrow 15$
$l = -13 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.082$
$S = 1.02$
3257 reflections
153 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0198P)^2 + 5.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.91$ 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 $^F2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $^F2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $^F2$ 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	0.97279 (3)	0.83837 (4)	0.46073 (4)	0.0385 (2)
Br2	0.97835 (3)	0.53826 (4)	0.22988 (4)	0.0411 (2)
Br3	0.79035 (4)	0.42511 (5)	0.56367 (6)	0.0626 (2)
Br4	0.69346 (4)	0.83661 (6)	0.25087 (6)	0.0621 (2)
O1	0.8645 (3)	0.7469 (4)	0.1800 (3)	0.0396 (11)
O2	0.9393 (2)	0.5910 (3)	0.5489 (3)	0.0416 (11)
C1	0.8691 (3)	0.7629 (4)	0.2944 (4)	0.0287 (12)
C2	0.9543 (3)	0.7447 (4)	0.3320 (4)	0.0303 (12)
C3	0.9735 (3)	0.6266 (4)	0.3647 (4)	0.0297 (11)
C4	0.9144 (3)	0.5721 (4)	0.4411 (4)	0.0295 (11)
C5	0.8294 (3)	0.6072 (3)	0.4220 (4)	0.0283 (12)
C6	0.7682 (3)	0.5481 (4)	0.4738 (4)	0.0403 (17)
C7	0.6890 (3)	0.5742 (5)	0.4602 (5)	0.0533 (19)
C8	0.6691 (3)	0.6602 (5)	0.3929 (5)	0.052 (2)
C9	0.7277 (3)	0.7192 (4)	0.3411 (4)	0.0383 (17)
C10	0.8075 (3)	0.6947 (3)	0.3542 (4)	0.0273 (12)
H1	0.85650	0.84070	0.30820	0.0340*
HO1	0.867 (6)	0.698 (6)	0.167 (7)	0.09 (4)*
H2	0.99070	0.76750	0.27430	0.0360*
HO2	0.916 (4)	0.630 (4)	0.563 (5)	0.036 (19)*
H3	1.02600	0.62550	0.39880	0.0360*
H4	0.91720	0.49230	0.42830	0.0350*
H7	0.64980	0.53420	0.49590	0.0640*
H8	0.61610	0.67860	0.38240	0.0620*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0441 (3)	0.0369 (2)	0.0346 (3)	−0.0062 (2)	−0.0047 (2)	−0.0034 (2)
Br2	0.0530 (3)	0.0353 (2)	0.0351 (3)	0.0038 (2)	0.0128 (2)	−0.0024 (2)
Br3	0.0734 (4)	0.0474 (3)	0.0669 (4)	−0.0074 (3)	0.0240 (3)	0.0210 (3)
Br4	0.0521 (3)	0.0739 (4)	0.0602 (4)	0.0243 (3)	−0.0131 (3)	0.0098 (3)
O1	0.047 (2)	0.047 (2)	0.0247 (18)	−0.0041 (19)	−0.0016 (15)	0.0047 (17)
O2	0.047 (2)	0.049 (2)	0.0289 (19)	0.0149 (19)	0.0012 (17)	0.0040 (17)
C1	0.032 (2)	0.027 (2)	0.027 (2)	−0.0020 (18)	−0.0029 (19)	0.0030 (17)
C2	0.029 (2)	0.034 (2)	0.028 (2)	−0.0012 (18)	0.0021 (18)	0.0018 (19)

C3	0.0240 (19)	0.035 (2)	0.030 (2)	0.0016 (18)	0.0039 (19)	−0.0009 (18)
C4	0.034 (2)	0.0274 (19)	0.027 (2)	0.0042 (18)	0.0075 (19)	0.0028 (18)
C5	0.030 (2)	0.028 (2)	0.027 (2)	0.0005 (17)	0.0040 (18)	−0.0011 (17)
C6	0.044 (3)	0.042 (3)	0.035 (3)	−0.003 (2)	0.009 (2)	0.002 (2)
C7	0.036 (3)	0.062 (3)	0.062 (4)	−0.016 (3)	0.012 (3)	−0.001 (3)
C8	0.026 (2)	0.070 (4)	0.060 (4)	−0.004 (3)	0.001 (2)	−0.004 (3)
C9	0.031 (3)	0.045 (3)	0.039 (3)	0.004 (2)	−0.004 (2)	−0.004 (2)
C10	0.026 (2)	0.030 (2)	0.026 (2)	0.0019 (17)	−0.0038 (18)	−0.0032 (17)

Geometric parameters (Å, º)

Br1—C2	1.978 (5)	C5—C10	1.400 (6)
Br2—C3	1.982 (5)	C5—C6	1.409 (7)
Br3—C6	1.895 (5)	C6—C7	1.382 (7)
Br4—C9	1.897 (5)	C7—C8	1.374 (9)
O1—C1	1.429 (6)	C8—C9	1.377 (7)
O2—C4	1.415 (6)	C9—C10	1.387 (7)
O1—HO1	0.62 (7)	C1—H1	0.9800
O2—HO2	0.64 (6)	C2—H2	0.9800
C1—C2	1.525 (7)	C3—H3	0.9800
C1—C10	1.518 (7)	C4—H4	0.9800
C2—C3	1.521 (7)	C7—H7	0.9300
C3—C4	1.523 (7)	C8—H8	0.9300
C4—C5	1.513 (7)		
Br1···O2	3.237 (4)	O2···Br1	3.237 (4)
Br1···C5	3.729 (4)	O2···Br3	3.220 (4)
Br1···Br2^{i}	3.6472 (7)	O2···C3^{iii}	3.200 (6)
Br1···Br2^{ii}	3.4762 (7)	O2···C4^{iii}	3.161 (6)
Br1···O1^{i}	3.426 (4)	O2···O1^{i}	2.840 (6)
Br2···O1	3.232 (5)	O1···HO2^{iv}	2.25 (6)
Br2···O2^{iii}	3.442 (4)	O2···H3^{iii}	2.7600
Br2···Br1^{iv}	3.6472 (7)	O2···H4^{iii}	2.6400
Br2···Br1^{v}	3.4762 (7)	C3···O2^{iii}	3.200 (6)
Br2···Br4^{vi}	3.7961 (9)	C4···O2^{iii}	3.161 (6)
Br3···O2	3.220 (4)	C5···Br1	3.729 (4)
Br3···C9^{vi}	3.725 (5)	C9···Br3^{vii}	3.725 (5)
Br4···O1	3.202 (5)	C6···HO2	2.90 (7)
Br4···Br2^{vii}	3.7961 (9)	H1···Br4	2.8400
Br1···H7^{vii}	3.1700	HO1···Br2	2.81 (9)
Br1···H8^{viii}	3.1000	HO1···Br1^{iv}	3.14 (9)
Br1···HO2	2.98 (5)	HO1···HO2^{iv}	2.58 (10)
Br1···HO1^{i}	3.14 (9)	HO2···Br1	2.98 (5)
Br2···H8^{ix}	3.1900	HO2···C6	2.90 (7)
Br2···HO1	2.81 (9)	HO2···O1^{i}	2.25 (6)
Br3···H3^{iii}	3.1900	HO2···HO1^{i}	2.58 (10)
Br3···H4	2.8300	H3···Br3^{iii}	3.1900
Br4···H1	2.8400	H3···O2^{iii}	2.7600

O1···Br2	3.232 (5)	H4···Br3	2.8300
O1···Br4	3.202 (5)	H4···O2^{iii}	2.6400
O1···Br1^{iv}	3.426 (4)	H7···Br1^{vi}	3.1700
O1···O2^{iv}	2.840 (6)	H8···Br1^{x}	3.1000
O2···Br2^{iii}	3.442 (4)	H8···Br2^{xi}	3.1900

C1—O1—HO1	113 (8)	Br4—C9—C10	121.6 (4)
C4—O2—HO2	101 (6)	C8—C9—C10	122.0 (5)
O1—C1—C2	109.4 (4)	Br4—C9—C8	116.4 (4)
O1—C1—C10	111.8 (4)	C5—C10—C9	119.2 (4)
C2—C1—C10	114.6 (4)	C1—C10—C5	121.5 (4)
Br1—C2—C1	108.1 (3)	C1—C10—C9	119.3 (4)
C1—C2—C3	114.7 (4)	O1—C1—H1	107.00
Br1—C2—C3	107.0 (3)	C2—C1—H1	107.00
Br2—C3—C4	108.3 (3)	C10—C1—H1	107.00
Br2—C3—C2	107.0 (3)	Br1—C2—H2	109.00
C2—C3—C4	115.7 (4)	C1—C2—H2	109.00
O2—C4—C5	112.5 (4)	C3—C2—H2	109.00
O2—C4—C3	108.6 (4)	Br2—C3—H3	108.00
C3—C4—C5	113.6 (4)	C2—C3—H3	109.00
C6—C5—C10	117.6 (5)	C4—C3—H3	109.00
C4—C5—C10	123.8 (4)	O2—C4—H4	107.00
C4—C5—C6	118.7 (4)	C3—C4—H4	107.00
Br3—C6—C5	121.4 (4)	C5—C4—H4	107.00
Br3—C6—C7	116.2 (4)	C6—C7—H7	121.00
C5—C6—C7	122.4 (5)	C8—C7—H7	121.00
C6—C7—C8	118.9 (5)	C7—C8—H8	120.00
C7—C8—C9	120.0 (5)	C9—C8—H8	120.00

C10—C1—C2—Br1	−83.3 (4)	C3—C4—C5—C10	−10.4 (6)
C10—C1—C2—C3	35.9 (6)	C4—C5—C10—C9	179.1 (4)
O1—C1—C2—C3	−90.5 (5)	C4—C5—C6—Br3	−1.2 (6)
C2—C1—C10—C9	168.1 (4)	C4—C5—C6—C7	−179.6 (5)
O1—C1—C2—Br1	150.3 (3)	C6—C5—C10—C9	0.0 (7)
O1—C1—C10—C5	113.0 (5)	C10—C5—C6—Br3	177.9 (3)
O1—C1—C10—C9	−66.7 (6)	C10—C5—C6—C7	−0.4 (7)
C2—C1—C10—C5	−12.2 (6)	C4—C5—C10—C1	−0.6 (7)
C1—C2—C3—Br2	72.5 (5)	C6—C5—C10—C1	−179.7 (4)
Br1—C2—C3—Br2	−167.7 (2)	C5—C6—C7—C8	0.7 (8)
Br1—C2—C3—C4	71.5 (5)	Br3—C6—C7—C8	−177.8 (5)
C1—C2—C3—C4	−48.3 (6)	C6—C7—C8—C9	−0.5 (9)
C2—C3—C4—O2	−91.5 (5)	C7—C8—C9—C10	0.1 (9)
Br2—C3—C4—C5	−85.6 (4)	C7—C8—C9—Br4	−179.7 (5)
Br2—C3—C4—O2	148.4 (3)	Br4—C9—C10—C5	179.9 (4)
C2—C3—C4—C5	34.5 (6)	Br4—C9—C10—C1	−0.4 (6)
C3—C4—C5—C6	168.7 (4)	C8—C9—C10—C5	0.1 (7)

O2—C4—C5—C6	−67.4 (5)	C8—C9—C10—C1	179.8 (5)
O2—C4—C5—C10	113.5 (5)		

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) −*x*+2, *y*+1/2, −*z*+1/2; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) *x*, −*y*+3/2, *z*−1/2; (v) −*x*+2, *y*−1/2, −*z*+1/2; (vi) −*x*+3/2, *y*−1/2, *z*; (vii) −*x*+3/2, *y*+1/2, *z*; (viii) *x*+1/2, −*y*+3/2, −*z*+1; (ix) *x*+1/2, *y*, −*z*+1/2; (x) *x*−1/2, −*y*+3/2, −*z*+1; (xi) *x*−1/2, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H*O*1···Br2	0.62 (7)	2.81 (9)	3.232 (5)	130 (10)
O2—H*O*2···O1^{i}	0.64 (6)	2.25 (6)	2.840 (6)	155 (7)

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