

rac-(9*R*,10*R*)-3,6,9,10-Tetrabromo-8,8-dimethyl-9,10-dihydro-2*H*,8*H*-pyrano[2,3-*f*]chromen-2-one (tetrabromoseselin): a photobiochemically active pyranocoumarin

A. K. Bauri,^a Sabine Foro^b and A. F. M. M. Rahman^{c*}

Received 22 February 2018

Accepted 28 February 2018

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; tetrabromoseselin; pyranocoumarin; bromination using bromine; photo-biochemical activity; hydrogen bonding; offset π - π interactions.

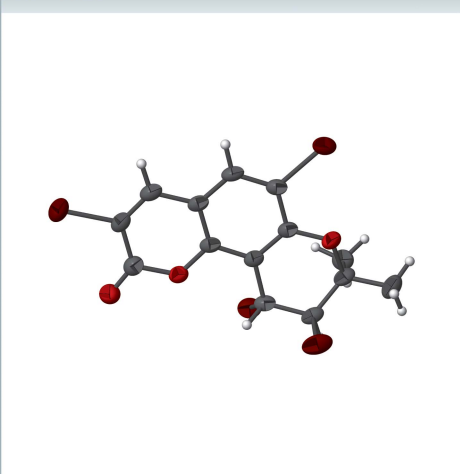
CCDC reference: 1826410

Structural data: full structural data are available from iucrdata.iucr.org

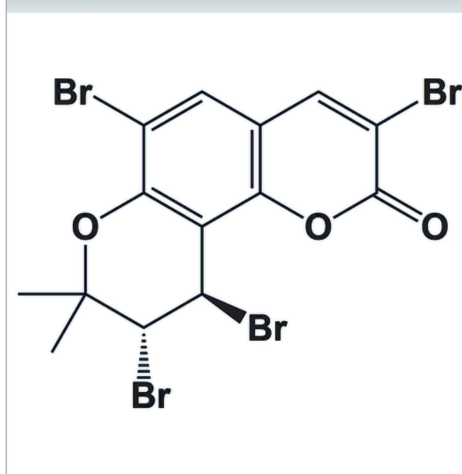
^aBio-Organic Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India, ^bInstitute of Materials Science, Darmstadt University of Technology, Alarich-Weiss-Strasse 2, D-64287 Darmstadt, Germany, and ^cDepartment of Applied Chemistry & Chemical Engineering, University of Dhaka, Dhaka-1000, Bangladesh. *Correspondence e-mail: mustafizacce@du.ac.bd

The title molecule, C₁₄H₁₀Br₄O₃, is a tetrabrominated substituted pyranocoumarin synthesized by bromination of seselin (systematic name: 8,8-dimethyl-2*H*,8*H*-pyrano[2,3-*f*]chromene-2-one) isolated from the Indian herb *Trachyspermum stictocapum*. The pyran ring has a distorted half-chair conformation and its mean plane is inclined to mean plane of the coumarin unit by 3.33 (17)°. In the crystal, molecules are linked by pairs of C—H...O hydrogen bonds, forming inversion dimers with an R₂²(16) ring motif. The dimers are linked by pairs of C—H...Br hydrogen bonds, enclosing an R₂²(16) ring motif, forming chains propagating along the [1 $\bar{1}$ 0] direction. Within the chains there are offset π - π interactions involving inversion-related benzene rings with an intercentroid distance of 3.788 (2) Å.

3D view



Chemical scheme



Structure description

The title compound (I) is a substituted angular pyranocoumarin derivative of seselin (II), whose crystal structure has previously been reported (Kato, 1970; Bauri *et al.*, 2006). We have described the properties of pyranocoumarins when reporting the crystal structures of 8,8-dimethyl-3,4,9,10-tetrahydro-2*H*,8*H*-pyrano[2,3-*f*]chromen-2-one [(III); Bauri *et al.*, 2017*a*], *rac*-(9*S*,10*R*)-3,9-dibromo-10-methoxy-8,8-dimethyl-9,10-dihydro-2*H*,8*H*-pyrano [2,3-*f*]chromen-2-one [(IV); Bauri *et al.*, 2017*b*], and *rac*-(9*S*,10*R*)-9-bromo-10-hydroxy-8,8-dimethyl-9,10-dihydro-2*H*,8*H*-pyrano [2,3-*f*]chromen-2-one [(V); Bauri *et al.*, 2017*c*] (Fig. 1).

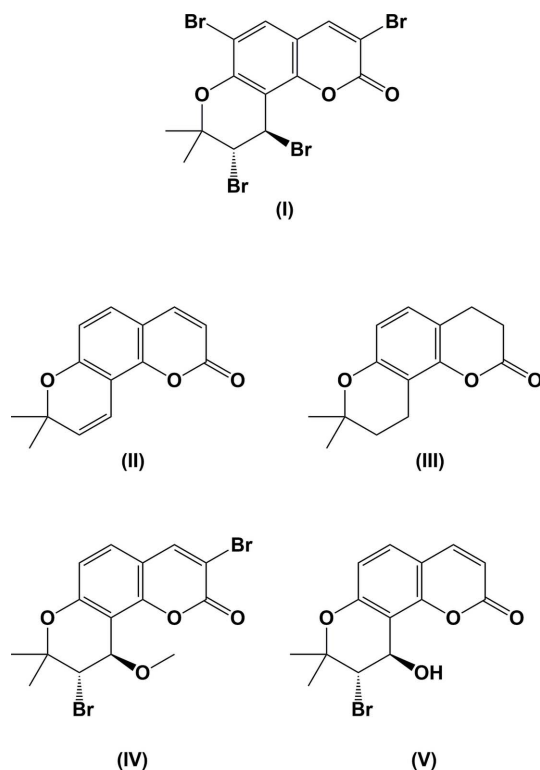


Figure 1
The title compound and related compounds.

The title molecule (I), illustrated in Fig. 2, belongs to a class of naturally occurring pyranocoumarins, known as psoralene. It is an angular isomer of the substituted pyranocoumarin seselin (II). It is composed of three rings, *viz.* a benzene and a pyrone ring each with one Br atom positioned at C12 and C8, respectively, and a pyran ring with a dimethyl-substituted C atom, C2, and two Br substituents located at positions C3 and C4; see Fig. 2. The C5–C6–C10–C11 and C5–C6–C10–C9 torsion angles are very similar [-0.8 (6) and -179.3 (4) $^\circ$, respectively) indicating that these rings are coplanar. The pyran ring (O1/C1–C5) has a distorted half-chair conformation [puckering parameters: $Q = 0.420$ (5) Å, $\theta = 129.9$ (7) $^\circ$, $\varphi =$

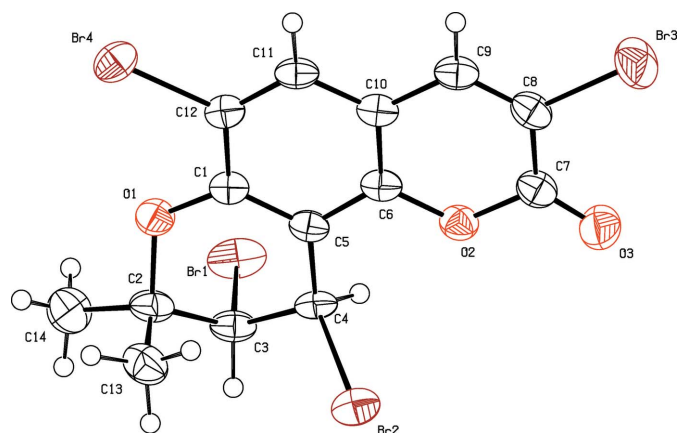


Figure 2
The molecular structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level

Table 1
Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3–H3 \cdots O3 ⁱ	0.98	2.43	3.277 (6)	144
C9–H9 \cdots Br1 ⁱⁱ	0.93	2.91	3.771 (5)	154

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

98.9 (8) $^\circ$], probably because of the ring flexibility and the presence of the substituents. Its mean plane is inclined to the mean plane of the coumarin ring system (O2/C1/C5–C12, r.m.s. deviation = 0.016 Å) by 3.33 (17) $^\circ$. There are two asymmetric centres at positions C3 and C4 (Fig. 1) and the present study indicates their relative configuration to be *R,R*.

In crystal, molecules are linked by pairs of C–H \cdots O hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif. Details of the hydrogen bonding are given in Table 1 and Fig. 3. The dimers are linked by pairs of C–H \cdots Br hydrogen bonds, enclosing an $R_2^2(16)$ ring motif, forming chains propagating along [1 $\bar{1}$ 0]. Within the chains there are offset π – π interactions involving inversion-related benzene rings (Fig. 2); $Cg\cdots Cg^{ii} = 3.788$ (2) Å, Cg is the centroid of ring C1/C5/C6/C10–C12, interplanar distance = 3.459 (2) Å, slippage = 1.544 Å; symmetry code: (ii) $-x, -y, -z$.

Synthesis and crystallization

The seselin synthon was isolated as a colourless crystalline solid from the methanol extract of *T. stictocurpum* by means of column chromatography (CC) over SiO₂ gel by gradient elution with a mixture of binary solvents (hexane and ethyl acetate). Finally it was purified by reverse-phase high-pressure liquid chromatography. It was then brominated in benzene under reflux conditions over a period of 12 h with continuous

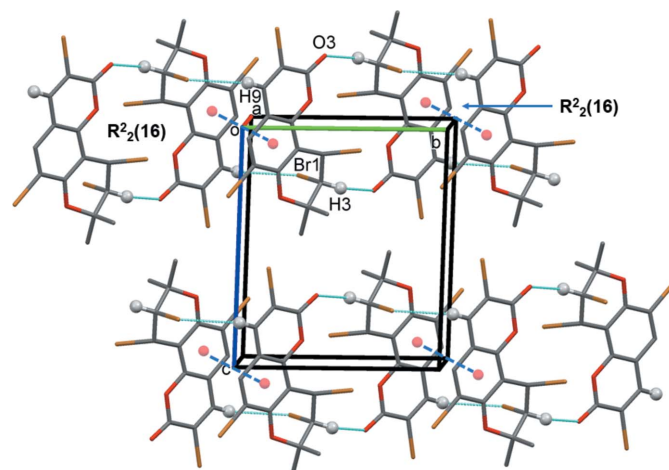


Figure 3
A view along the *a* axis of the crystal packing of the title compound, showing the hydrogen bonds (dashed cyan lines; see Table 1), the offset π – π interactions (blue dashed lines), and indicating the $R_2^2(16)$ ring motifs in the hydrogen-bonded chain. Only H atoms H3 and H9 have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₁₀ Br ₄ O ₃
<i>M</i> _r	545.86
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	299
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.2256 (8), 10.4409 (9), 11.2102 (9)
α , β , γ (°)	91.337 (7), 93.972 (8), 110.077 (9)
<i>V</i> (Å ³)	791.41 (13)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	10.18
Crystal size (mm)	0.40 × 0.24 × 0.12
Data collection	
Diffractometer	Oxford Diffraction Xcalibur with a Sapphire CCD detector
Absorption correction	Multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2009)
<i>T</i> _{min} , <i>T</i> _{max}	0.106, 0.375
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	4887, 2870, 2365
<i>R</i> _{int}	0.015
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.602
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.033, 0.091, 1.06
No. of reflections	2870
No. of parameters	192
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.76, -0.65

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

stirring. The crude brominated seselin was purified by CC over SiO₂ by gradient solvent elution and crystallized as colourless crystals. Crystals suitable for X-ray diffraction analysis were obtained by recrystallization (× 3) from an ethyl acet-

ate:hexane (1:4) solution at room temperature by slow evaporation of the solvents. Spectroscopic data: ¹H NMR (CDCl₃, 200 MHz): δ_{H} 7.11 (*s*, 1H, H-9), 7.05 (*s*, 1H, H-9), 5.25 (*d*, 1H, *J* = 9.8 Hz, H-4), 4.26 (*d*, 1H, *J* = 9.8 Hz, H-3), 1.50 (*s*, 3H, CH₃, H-13), 1.54 (*s*, 3H, CH₃, H-14).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank Professor Dr Hartmut, FG Struktur-forschung, Material-und Geowissenschaften, Technische Universität Darmstadt, for his kind co-operation to record the XRD of the crystal and provide diffractometer time.

References

- Bauri, A. K., Foro, S., Lindner, H.-J. & Nayak, S. K. (2006). *Acta Cryst.* **E62**, o1340–o1341.
- Bauri, A. K., Foro, S. & Rahman, A. F. M. M. (2017a). *Acta Cryst.* **E73**, 1117–1120.
- Bauri, A. K., Foro, S. & Rahman, A. F. M. M. (2017b). *Acta Cryst.* **E73**, 774–776.
- Bauri, A. K., Foro, S. & Rahman, A. F. M. M. (2017c). *Acta Cryst.* **E73**, 453–455.
- Kato, K. (1970). *Acta Cryst.* **B26**, 2022–2029.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd., Abingdon, England.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

full crystallographic data

IUCrData (2018). 3, x180346 [https://doi.org/10.1107/S2414314618003462]

***rac*-(9*R*,10*R*)-3,6,9,10-Tetrabromo-8,8-dimethyl-9,10-dihydro-2*H*,8*H*-pyrano[2,3-*f*]chromen-2-one (tetrabromoseselin): a photobiochemically active pyranocoumarin**

A. K. Bauri, Sabine Foro and A. F. M. M. Rahman

rac-(9*R*,10*R*)-3,6,9,10-Tetrabromo-8,8-dimethyl-9,10-dihydro-2*H*,8*H*-pyrano[2,3-*f*]chromen-2-one

Crystal data

C₁₄H₁₀Br₄O₃

M_r = 545.86

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

a = 7.2256 (8) Å

b = 10.4409 (9) Å

c = 11.2102 (9) Å

α = 91.337 (7)°

β = 93.972 (8)°

γ = 110.077 (9)°

V = 791.41 (13) Å³

Z = 2

F(000) = 516

D_x = 2.291 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3670 reflections

θ = 2.7–27.8°

μ = 10.18 mm⁻¹

T = 299 K

Prism, colourless

0.40 × 0.24 × 0.12 mm

Data collection

Oxford Diffraction Xcalibur with a Sapphire

CCD detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using ω scans

Absorption correction: multi-scan

(CrysAlis RED; Oxford Diffraction, 2009)

T_{min} = 0.106, *T_{max}* = 0.375

4887 measured reflections

2870 independent reflections

2365 reflections with *I* > 2σ(*I*)

R_{int} = 0.015

θ_{\max} = 25.4°, θ_{\min} = 2.7°

h = -8→8

k = -12→12

l = -13→13

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.033

wR(*F*²) = 0.091

S = 1.06

2870 reflections

192 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/[σ²(*F_o*²) + (0.0513*P*)² + 1.0324*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.76 e Å⁻³

Δρ_{min} = -0.65 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 $F^2 \geq 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.56855 (7)	0.25787 (5)	0.22289 (6)	0.05285 (18)
Br2	0.28329 (8)	0.56363 (5)	0.10391 (5)	0.04718 (16)
Br3	-0.21257 (9)	0.16052 (7)	-0.42181 (5)	0.0626 (2)
Br4	-0.25882 (7)	-0.04642 (5)	0.27392 (5)	0.04240 (15)
O1	0.1145 (4)	0.1914 (3)	0.2955 (3)	0.0374 (7)
O2	0.1306 (4)	0.3208 (3)	-0.1092 (3)	0.0350 (7)
O3	0.1571 (5)	0.3827 (4)	-0.2955 (3)	0.0515 (9)
C1	0.0368 (6)	0.1798 (4)	0.1818 (4)	0.0297 (9)
C2	0.2614 (7)	0.3222 (5)	0.3396 (4)	0.0384 (11)
C3	0.4094 (6)	0.3763 (4)	0.2449 (4)	0.0353 (10)
H3	0.4986	0.4682	0.2714	0.042*
C4	0.3143 (6)	0.3823 (4)	0.1214 (4)	0.0309 (9)
H4	0.4059	0.3748	0.0633	0.037*
C5	0.1244 (6)	0.2667 (4)	0.0927 (4)	0.0296 (9)
C6	0.0364 (6)	0.2367 (4)	-0.0234 (4)	0.0301 (9)
C7	0.0616 (7)	0.3029 (5)	-0.2292 (4)	0.0373 (10)
C8	-0.1199 (7)	0.1882 (5)	-0.2591 (4)	0.0371 (10)
C9	-0.2127 (6)	0.1043 (5)	-0.1773 (4)	0.0355 (10)
H9	-0.3276	0.0310	-0.2000	0.043*
C10	-0.1349 (6)	0.1271 (4)	-0.0539 (4)	0.0302 (9)
C11	-0.2222 (6)	0.0418 (4)	0.0367 (4)	0.0327 (10)
H11	-0.3374	-0.0329	0.0186	0.039*
C12	-0.1377 (6)	0.0685 (4)	0.1513 (4)	0.0313 (9)
C13	0.1523 (8)	0.4204 (5)	0.3642 (5)	0.0475 (12)
H13A	0.0685	0.4222	0.2944	0.057*
H13B	0.2465	0.5103	0.3832	0.057*
H13C	0.0733	0.3906	0.4304	0.057*
C14	0.3513 (8)	0.2900 (6)	0.4562 (5)	0.0554 (14)
H14A	0.2514	0.2607	0.5118	0.066*
H14B	0.4558	0.3702	0.4892	0.066*
H14C	0.4035	0.2185	0.4415	0.066*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0330 (3)	0.0397 (3)	0.0876 (4)	0.0167 (2)	-0.0031 (2)	-0.0027 (3)
Br2	0.0460 (3)	0.0335 (3)	0.0621 (3)	0.0138 (2)	0.0052 (2)	0.0015 (2)
Br3	0.0543 (4)	0.0749 (4)	0.0411 (3)	0.0033 (3)	-0.0118 (2)	-0.0006 (3)
Br4	0.0317 (3)	0.0387 (3)	0.0537 (3)	0.0073 (2)	0.0061 (2)	0.0093 (2)
O1	0.0309 (16)	0.0365 (17)	0.0376 (18)	0.0042 (13)	-0.0048 (13)	0.0007 (13)
O2	0.0293 (16)	0.0340 (16)	0.0371 (17)	0.0057 (13)	0.0006 (13)	-0.0024 (13)
O3	0.045 (2)	0.052 (2)	0.045 (2)	0.0008 (17)	0.0019 (16)	0.0053 (17)
C1	0.023 (2)	0.028 (2)	0.039 (2)	0.0095 (17)	0.0019 (17)	-0.0019 (18)
C2	0.032 (2)	0.030 (2)	0.046 (3)	0.0044 (19)	-0.008 (2)	-0.007 (2)
C3	0.026 (2)	0.027 (2)	0.051 (3)	0.0089 (18)	-0.0059 (19)	-0.0063 (19)
C4	0.026 (2)	0.0198 (19)	0.046 (3)	0.0073 (17)	0.0037 (18)	-0.0036 (18)
C5	0.025 (2)	0.027 (2)	0.038 (2)	0.0113 (17)	0.0013 (17)	-0.0051 (18)
C6	0.022 (2)	0.027 (2)	0.042 (2)	0.0098 (17)	0.0035 (18)	-0.0047 (18)
C7	0.036 (2)	0.038 (2)	0.039 (3)	0.015 (2)	0.000 (2)	-0.004 (2)
C8	0.033 (2)	0.041 (3)	0.037 (2)	0.015 (2)	-0.0050 (19)	-0.007 (2)
C9	0.026 (2)	0.031 (2)	0.047 (3)	0.0092 (18)	-0.0032 (19)	-0.005 (2)
C10	0.022 (2)	0.028 (2)	0.042 (3)	0.0112 (17)	-0.0002 (18)	-0.0046 (18)
C11	0.021 (2)	0.026 (2)	0.048 (3)	0.0052 (17)	0.0001 (18)	-0.0047 (19)
C12	0.024 (2)	0.028 (2)	0.042 (3)	0.0090 (17)	0.0058 (18)	-0.0002 (18)
C13	0.046 (3)	0.049 (3)	0.046 (3)	0.015 (2)	0.007 (2)	-0.009 (2)
C14	0.053 (3)	0.057 (3)	0.046 (3)	0.010 (3)	-0.017 (2)	0.002 (3)

Geometric parameters (\AA , $^\circ$)

Br1—C3	1.979 (4)	C4—H4	0.9800
Br2—C4	1.994 (4)	C5—C6	1.388 (6)
Br3—C8	1.879 (5)	C6—C10	1.382 (6)
Br4—C12	1.902 (4)	C7—C8	1.452 (6)
O1—C1	1.342 (5)	C8—C9	1.334 (7)
O1—C2	1.462 (5)	C9—C10	1.439 (6)
O2—C6	1.371 (5)	C9—H9	0.9300
O2—C7	1.387 (5)	C10—C11	1.403 (6)
O3—C7	1.196 (6)	C11—C12	1.364 (6)
C1—C5	1.399 (6)	C11—H11	0.9300
C1—C12	1.405 (6)	C13—H13A	0.9600
C2—C14	1.515 (7)	C13—H13B	0.9600
C2—C13	1.523 (7)	C13—H13C	0.9600
C2—C3	1.537 (7)	C14—H14A	0.9600
C3—C4	1.514 (6)	C14—H14B	0.9600
C3—H3	0.9800	C14—H14C	0.9600
C4—C5	1.492 (6)		
C1—O1—C2	118.3 (3)	O3—C7—C8	127.6 (4)
C6—O2—C7	123.1 (3)	O2—C7—C8	115.5 (4)
O1—C1—C5	124.0 (4)	C9—C8—C7	122.4 (4)

O1—C1—C12	116.7 (4)	C9—C8—Br3	121.6 (4)
C5—C1—C12	119.2 (4)	C7—C8—Br3	116.0 (3)
O1—C2—C14	104.1 (4)	C8—C9—C10	120.0 (4)
O1—C2—C13	107.8 (4)	C8—C9—H9	120.0
C14—C2—C13	109.9 (4)	C10—C9—H9	120.0
O1—C2—C3	109.3 (4)	C6—C10—C11	118.3 (4)
C14—C2—C3	114.4 (4)	C6—C10—C9	118.5 (4)
C13—C2—C3	110.9 (4)	C11—C10—C9	123.2 (4)
C4—C3—C2	114.2 (4)	C12—C11—C10	119.8 (4)
C4—C3—Br1	105.2 (3)	C12—C11—H11	120.1
C2—C3—Br1	111.2 (3)	C10—C11—H11	120.1
C4—C3—H3	108.7	C11—C12—C1	121.7 (4)
C2—C3—H3	108.7	C11—C12—Br4	119.6 (3)
Br1—C3—H3	108.7	C1—C12—Br4	118.8 (3)
C5—C4—C3	112.7 (4)	C2—C13—H13A	109.5
C5—C4—Br2	112.3 (3)	C2—C13—H13B	109.5
C3—C4—Br2	109.8 (3)	H13A—C13—H13B	109.5
C5—C4—H4	107.2	C2—C13—H13C	109.5
C3—C4—H4	107.2	H13A—C13—H13C	109.5
Br2—C4—H4	107.2	H13B—C13—H13C	109.5
C6—C5—C1	118.0 (4)	C2—C14—H14A	109.5
C6—C5—C4	121.5 (4)	C2—C14—H14B	109.5
C1—C5—C4	120.4 (4)	H14A—C14—H14B	109.5
O2—C6—C10	120.6 (4)	C2—C14—H14C	109.5
O2—C6—C5	116.4 (4)	H14A—C14—H14C	109.5
C10—C6—C5	123.0 (4)	H14B—C14—H14C	109.5
O3—C7—O2	116.8 (4)		
C2—O1—C1—C5	19.7 (6)	C4—C5—C6—O2	-1.6 (6)
C2—O1—C1—C12	-163.7 (4)	C1—C5—C6—C10	1.4 (6)
C1—O1—C2—C14	-166.8 (4)	C4—C5—C6—C10	177.3 (4)
C1—O1—C2—C13	76.5 (5)	C6—O2—C7—O3	-179.8 (4)
C1—O1—C2—C3	-44.2 (5)	C6—O2—C7—C8	0.3 (6)
O1—C2—C3—C4	52.5 (5)	O3—C7—C8—C9	179.1 (5)
C14—C2—C3—C4	168.7 (4)	O2—C7—C8—C9	-1.0 (7)
C13—C2—C3—C4	-66.3 (5)	O3—C7—C8—Br3	1.2 (7)
O1—C2—C3—Br1	-66.3 (4)	O2—C7—C8—Br3	-178.9 (3)
C14—C2—C3—Br1	49.9 (5)	C7—C8—C9—C10	1.0 (7)
C13—C2—C3—Br1	174.9 (3)	Br3—C8—C9—C10	178.7 (3)
C2—C3—C4—C5	-35.9 (5)	O2—C6—C10—C11	178.1 (4)
Br1—C3—C4—C5	86.3 (4)	C5—C6—C10—C11	-0.8 (6)
C2—C3—C4—Br2	90.2 (4)	O2—C6—C10—C9	-0.5 (6)
Br1—C3—C4—Br2	-147.7 (2)	C5—C6—C10—C9	-179.3 (4)
O1—C1—C5—C6	175.0 (4)	C8—C9—C10—C6	-0.2 (6)
C12—C1—C5—C6	-1.6 (6)	C8—C9—C10—C11	-178.7 (4)
O1—C1—C5—C4	-0.9 (6)	C6—C10—C11—C12	0.2 (6)
C12—C1—C5—C4	-177.4 (4)	C9—C10—C11—C12	178.7 (4)
C3—C4—C5—C6	-165.9 (4)	C10—C11—C12—C1	-0.4 (7)

Br2—C4—C5—C6	69.4 (5)	C10—C11—C12—Br4	179.2 (3)
C3—C4—C5—C1	9.8 (6)	O1—C1—C12—C11	-175.7 (4)
Br2—C4—C5—C1	-114.9 (4)	C5—C1—C12—C11	1.1 (6)
C7—O2—C6—C10	0.4 (6)	O1—C1—C12—Br4	4.7 (5)
C7—O2—C6—C5	179.4 (4)	C5—C1—C12—Br4	-178.5 (3)
C1—C5—C6—O2	-177.4 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C3—H3...O3 ⁱ	0.98	2.43	3.277 (6)	144
C9—H9...Br1 ⁱⁱ	0.93	2.91	3.771 (5)	154

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