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2,7-Dibromo-10′*H*-spiro[fluorene-9,9′-phenanthren]-10′-one

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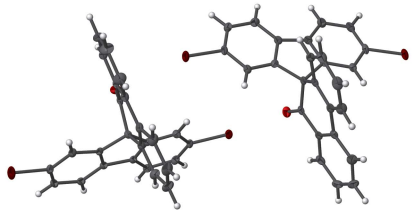
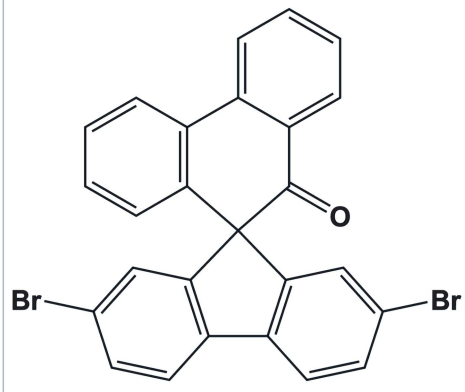
Structural data: full structural data are available from iucrdata.iucr.org

The title racemic spiro compound, $C_{26}H_{14}Br_2O$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The mean plane of the phenanthrene unit is twisted with respect to the mean plane of the fluorene unit by 82.38 (15) and 80.25 (5)° in molecules *A* and *B*, respectively. In the crystal, the *A* and *B* molecules are linked by a pair of C—H···O hydrogen bonds and a pair of short Br···O contacts [2.935 (2) Å], forming a centrosymmetric four-molecule unit. These units are linked by C—H···π interactions, forming ribbons propagating along the *b*-axis direction. The ribbons are linked by C—Br···π interactions, forming layers parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

The parent structure, 10′*H*-spiro[fluorene-9,9′-phenanthren]-10′-one and its analogues have been studied for the reactivity of fluorene (Suzuki *et al.* 1962). They are also of interest as building blocks for the preparation of microporous materials (Taylor *et al.* 2016) and for their electro-chemical properties (Debroy *et al.* 2007). Synthetic methods and physical properties of brominated 10′*H*-spiro[fluorene-9,9′-phenanthren]-10′-one compounds have been reported (Suzuki *et al.*, 1962; Borowitz *et al.*, 1971). Herein, we report on the high-yield synthesis and the crystal structure of the title racemic spiro compound, which to the best of our knowledge is a unique example of this type of compound.

The title compound, illustrated in Fig. 1, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. In molecule *A*, the mean plane of the fluorene unit (r.m.s. deviation = 0.02 Å) is inclined to the mean plane of the phenanthrene unit (r.m.s. deviation = 0.096 Å) by 82.38 (5)°. In molecule *B*, the corresponding angle is 80.25 (5)°

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

*Cg*2, *Cg*3, *Cg*6, *Cg*15 and *Cg*17 are the centroids of the C1–C3/C8/C9/C14, C3–C8, C21–C26, C29–C24 and C41–C46 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C44—H44···O1^{i}	0.95	2.44	3.364 (3)	163
C5—H5···*Cg*6^{ii}	0.95	2.69	3.554 (3)	151
C31—H31···*Cg*17^{iii}	0.95	2.88	3.780 (3)	158
C24—Br2···*Cg*15^{iv}	1.90 (1)	3.44 (1)	5.330 (3)	173 (1)
C50—Br4···*Cg*2	1.91 (1)	3.78 (1)	5.454 (3)	145 (1)
C50—Br4···*Cg*3	1.91 (1)	3.91 (1)	5.790 (3)	168 (1)

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

(r.m.s. deviations are 0.02 and 0.123 Å, respectively), indicating that the conformation of the two molecules is very similar.

In the crystal, the *A* and *B* molecules are linked by a pair of C—H···O hydrogen bonds and a pair of short Br···O contacts [2.935 (2) Å], forming a centrosymmetric four-molecule unit (Table 1 and Fig. 2). These units are linked by C—H···π interactions, forming ribbons along the *b* axis direction (Table 1 and Fig. 3). The ribbons are linked by C—Br···π interactions, forming layers parallel to the *ab* plane (Table 1 and Fig. 4).

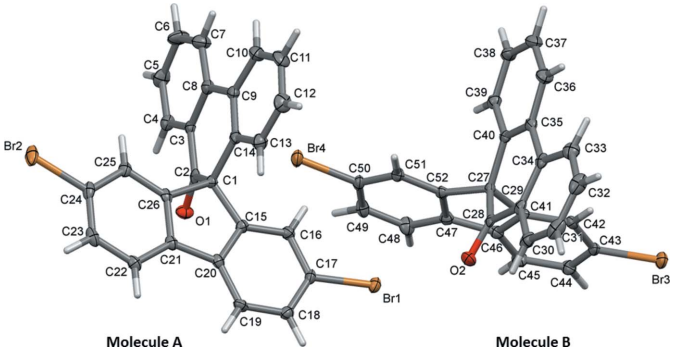


Figure 1
The molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

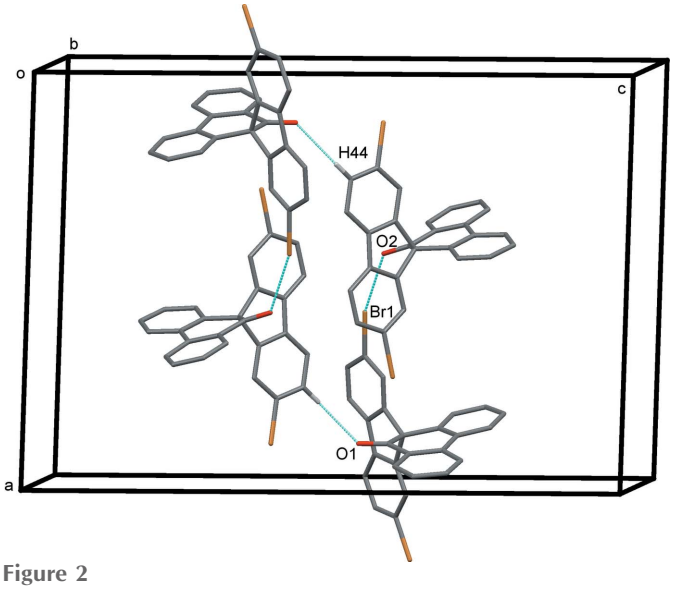


Figure 2
A view along the *b* axis of the centrosymmetric four-molecule unit, formed by C—H···O hydrogen bonds (see Table 1) and short Br···O contacts [2.935 (2) Å]. For clarity, only H atom H44 has been included.

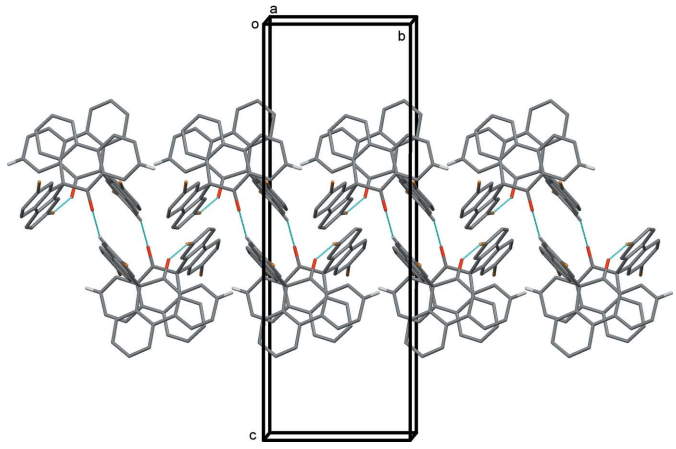


Figure 3
A view along the *a* axis of the ribbons formed by the C—H···π interactions (see Table 1) that link the centrosymmetric four-molecule units. For clarity, only H atoms H44, H5 and H31 have been included.

Synthesis and crystallization

The title compound was synthesized from the reaction of 10′*H*-spiro[fluorene-9,9′-phenanthren]-10′-one (1 mg, 2.9 mmol) and bromine (0.4 ml, 7.76 mmol) in dichloromethane at room temperature (86% yield). Colourless plate-like crystals of the title compound were grown by slow evaporation, at room temperature, of a solution in dichloro-

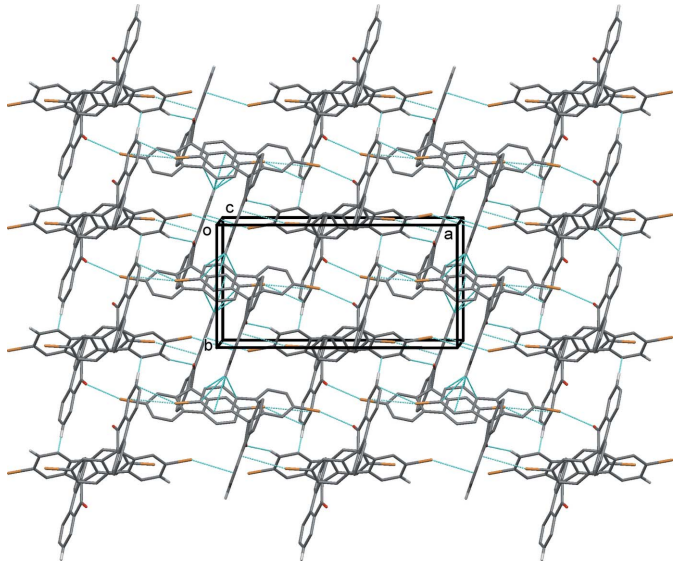


Figure 4
A view along the *c* axis of the crystal packing of the title compound. The various intermolecular contacts are illustrated by single or mulitple dashed lines (see Table 1). For clarity, only H atoms H44, H5 and H31 have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{14}Br_2O$
M_r	502.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	17.511 (1), 8.9191 (7), 25.2761 (15)
β (°)	92.179 (2)
V (Å^3)	3944.8 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.13
Crystal size (mm)	0.44 × 0.30 × 0.26
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.640, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	122604, 8667, 7162
R_{int}	0.072
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.640
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.063, 1.03
No. of reflections	8667
No. of parameters	523
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.46, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2001), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2013* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008) and *WinGX* (Farrugia, 2012).

methane (m.p. 533–535 K). ^{1}H (400 MHz, $CDCl_3$): δ 8.22 (*d*, 1H, J = 8.12 Hz), 8.14 (*d*, 1H, J = 7.8 Hz), 8.03 (*dd*, 1H, J = 7.76, 1.32 Hz), 7.84 (*t*, 1H, J = 7.92 Hz), 7.66 (*s*, 1H), 7.64 (*s*, 1H), 7.49–7.55 (*m*, 3H), 7.43 (*t*, 1H, J = 7.86 Hz), 7.13–7.17 (*m*, 3H), 6.59 (*dd*, 1H, J = 7.88, 1.12 Hz). ^{13}C (100 MHz, $CDCl_3$): δ 195.7, 149.1, 139.6, 137.7, 137.5, 135.4, 131.7, 130.3, 129.5, 129.3, 128.8, 128.7, 128.6, 128.2, 127.9, 124.3, 123.4, 121.9, 121.8.

Refinement

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

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full crystallographic data

IUCrData (2017). **2**, x170301 [https://doi.org/10.1107/S2414314617003017]

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Crystal data

$C_{26}H_{14}Br_2O$
M_r = 502.19
Monoclinic, $P2_1/c$
a = 17.511 (1) Å
b = 8.9191 (7) Å
c = 25.2761 (15) Å
β = 92.179 (2)°
V = 3944.8 (4) Å^3
Z = 8
$F(000)$ = 1984
D_x = 1.691 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9798 reflections
θ = 2.7–27.1°
μ = 4.13 mm^{-1}
T = 100 K
Prism, colourless
0.44 × 0.30 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.640, T_{max} = 0.971
122604 measured reflections
8667 independent reflections
7162 reflections with $I > 2\sigma(I)$
R_{int} = 0.072
θ_{max} = 27.1°, θ_{min} = 2.0°
h = −22→22
k = −11→11
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.063
S = 1.03
8667 reflections
523 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
$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2 + 4.6257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.58632 (2)	0.45391 (3)	0.53916 (2)	0.01768 (6)
Br2	1.17959 (2)	0.52190 (3)	0.62371 (2)	0.02688 (7)
O1	0.88959 (10)	0.17311 (18)	0.55147 (6)	0.0196 (4)
C1	0.87687 (13)	0.3717 (2)	0.61400 (9)	0.0135 (5)
C2	0.89106 (13)	0.2074 (2)	0.59816 (9)	0.0140 (5)
C3	0.91023 (12)	0.0977 (3)	0.64026 (9)	0.0139 (5)
C4	0.93583 (13)	−0.0449 (3)	0.62497 (10)	0.0178 (5)
H4	0.9399	−0.0677	0.5885	0.021*
C5	0.95512 (15)	−0.1518 (3)	0.66266 (10)	0.0239 (6)
H5	0.9726	−0.2479	0.6523	0.029*
C6	0.94871 (16)	−0.1173 (3)	0.71570 (11)	0.0288 (6)
H6	0.9623	−0.1903	0.7418	0.035*
C7	0.92282 (16)	0.0221 (3)	0.73140 (10)	0.0261 (6)
H7	0.9186	0.0429	0.7680	0.031*
C8	0.90270 (13)	0.1329 (3)	0.69407 (9)	0.0171 (5)
C9	0.87267 (13)	0.2809 (3)	0.70961 (9)	0.0163 (5)
C10	0.85475 (15)	0.3109 (3)	0.76247 (10)	0.0234 (6)
H10	0.8625	0.2351	0.7885	0.028*
C11	0.82627 (16)	0.4481 (3)	0.77695 (10)	0.0274 (6)
H11	0.8144	0.4656	0.8128	0.033*
C12	0.81468 (16)	0.5607 (3)	0.74001 (10)	0.0272 (6)
H12	0.7955	0.6555	0.7503	0.033*
C13	0.83150 (14)	0.5335 (3)	0.68758 (10)	0.0218 (5)
H13	0.8236	0.6103	0.6619	0.026*
C14	0.85986 (13)	0.3944 (3)	0.67232 (9)	0.0149 (5)
C15	0.81596 (13)	0.4414 (2)	0.57728 (9)	0.0139 (5)
C16	0.73893 (13)	0.4104 (3)	0.57548 (9)	0.0155 (5)
H16	0.7181	0.3371	0.5981	0.019*
C17	0.69262 (13)	0.4903 (3)	0.53939 (9)	0.0153 (5)
C18	0.72257 (14)	0.5961 (3)	0.50532 (9)	0.0171 (5)
H18	0.6899	0.6465	0.4802	0.021*
C19	0.80014 (14)	0.6276 (3)	0.50815 (9)	0.0164 (5)
H19	0.8210	0.7007	0.4855	0.020*
C20	0.84714 (13)	0.5506 (3)	0.54469 (9)	0.0150 (5)
C21	0.92914 (13)	0.5620 (2)	0.55759 (9)	0.0144 (5)
C22	0.98559 (13)	0.6525 (3)	0.53700 (9)	0.0170 (5)
H22	0.9732	0.7227	0.5097	0.020*
C23	1.06016 (14)	0.6384 (3)	0.55690 (10)	0.0201 (5)
H23	1.0994	0.6990	0.5432	0.024*
C24	1.07723 (13)	0.5356 (3)	0.59686 (10)	0.0187 (5)
C25	1.02210 (13)	0.4439 (3)	0.61843 (9)	0.0168 (5)
H25	1.0348	0.3738	0.6457	0.020*
C26	0.94788 (13)	0.4597 (2)	0.59830 (9)	0.0144 (5)
Br3	0.11825 (2)	0.06102 (3)	0.58188 (2)	0.02152 (6)
Br4	0.72200 (2)	−0.00951 (3)	0.61494 (2)	0.02122 (6)

O2	0.44110 (9)	0.33247 (19)	0.57462 (6)	0.0209 (4)
C27	0.42160 (12)	0.1372 (2)	0.63726 (9)	0.0126 (4)
C28	0.42082 (12)	0.3019 (3)	0.61883 (9)	0.0141 (5)
C29	0.38932 (13)	0.4159 (3)	0.65432 (9)	0.0155 (5)
C30	0.37581 (14)	0.5601 (3)	0.63376 (10)	0.0212 (5)
H30	0.3881	0.5825	0.5983	0.025*
C31	0.34463 (15)	0.6697 (3)	0.66509 (11)	0.0257 (6)
H31	0.3355	0.7674	0.6513	0.031*
C32	0.32685 (15)	0.6360 (3)	0.71668 (11)	0.0265 (6)
H32	0.3054	0.7111	0.7382	0.032*
C33	0.34006 (15)	0.4940 (3)	0.73721 (10)	0.0229 (5)
H33	0.3269	0.4728	0.7725	0.028*
C34	0.37253 (13)	0.3811 (3)	0.70678 (9)	0.0166 (5)
C35	0.39221 (13)	0.2317 (3)	0.72944 (9)	0.0151 (5)
C36	0.38903 (15)	0.2040 (3)	0.78410 (10)	0.0231 (6)
H36	0.3728	0.2818	0.8068	0.028*
C37	0.40892 (15)	0.0663 (3)	0.80551 (10)	0.0251 (6)
H37	0.4060	0.0497	0.8425	0.030*
C38	0.43320 (14)	−0.0476 (3)	0.77287 (10)	0.0218 (5)
H38	0.4465	−0.1427	0.7874	0.026*
C39	0.43804 (13)	−0.0223 (3)	0.71900 (9)	0.0174 (5)
H39	0.4554	−0.1003	0.6968	0.021*
C40	0.41770 (13)	0.1161 (3)	0.69691 (9)	0.0138 (5)
C41	0.35281 (13)	0.0666 (2)	0.60646 (9)	0.0137 (5)
C42	0.27603 (13)	0.0989 (3)	0.61086 (9)	0.0151 (5)
H42	0.2590	0.1693	0.6361	0.018*
C43	0.22452 (13)	0.0234 (3)	0.57650 (9)	0.0165 (5)
C44	0.24804 (14)	−0.0779 (3)	0.53878 (9)	0.0202 (5)
H44	0.2115	−0.1262	0.5158	0.024*
C45	0.32557 (14)	−0.1082 (3)	0.53493 (10)	0.0207 (5)
H45	0.3425	−0.1773	0.5093	0.025*
C46	0.37807 (14)	−0.0363 (3)	0.56894 (9)	0.0160 (5)
C47	0.46145 (13)	−0.0465 (3)	0.57357 (9)	0.0162 (5)
C48	0.51275 (14)	−0.1339 (3)	0.54643 (10)	0.0219 (5)
H48	0.4950	−0.2014	0.5196	0.026*
C49	0.59027 (14)	−0.1209 (3)	0.55918 (10)	0.0212 (5)
H49	0.6262	−0.1797	0.5411	0.025*
C50	0.61495 (13)	−0.0219 (3)	0.59844 (10)	0.0171 (5)
C51	0.56498 (13)	0.0679 (3)	0.62596 (9)	0.0155 (5)
H51	0.5831	0.1360	0.6525	0.019*
C52	0.48773 (13)	0.0537 (2)	0.61306 (9)	0.0142 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01159 (11)	0.02131 (12)	0.01997 (12)	0.00043 (9)	−0.00161 (9)	−0.00174 (9)
Br2	0.01206 (12)	0.04248 (16)	0.02601 (14)	−0.00319 (11)	−0.00067 (10)	−0.01276 (12)
O1	0.0257 (9)	0.0190 (8)	0.0141 (8)	0.0006 (7)	−0.0001 (7)	−0.0026 (7)

C1	0.0126 (11)	0.0148 (11)	0.0129 (11)	−0.0016 (9)	0.0004 (9)	0.0004 (9)
C2	0.0081 (11)	0.0158 (11)	0.0182 (12)	−0.0033 (9)	0.0005 (9)	−0.0005 (9)
C3	0.0085 (11)	0.0165 (11)	0.0166 (11)	−0.0018 (9)	−0.0001 (9)	0.0005 (9)
C4	0.0154 (12)	0.0177 (12)	0.0200 (12)	0.0006 (10)	−0.0003 (10)	−0.0024 (10)
C5	0.0239 (14)	0.0147 (12)	0.0331 (15)	0.0052 (10)	0.0000 (11)	0.0007 (10)
C6	0.0375 (16)	0.0235 (14)	0.0249 (14)	0.0085 (12)	−0.0043 (12)	0.0075 (11)
C7	0.0339 (15)	0.0270 (14)	0.0175 (13)	0.0041 (12)	0.0013 (11)	0.0026 (11)
C8	0.0133 (12)	0.0197 (12)	0.0181 (12)	−0.0008 (9)	0.0000 (9)	0.0014 (10)
C9	0.0120 (11)	0.0218 (12)	0.0152 (12)	0.0000 (9)	0.0008 (9)	−0.0002 (9)
C10	0.0242 (14)	0.0306 (14)	0.0155 (12)	0.0035 (11)	0.0032 (10)	0.0002 (10)
C11	0.0281 (15)	0.0379 (16)	0.0167 (12)	0.0029 (12)	0.0073 (11)	−0.0056 (11)
C12	0.0296 (15)	0.0265 (14)	0.0256 (14)	0.0069 (12)	0.0035 (11)	−0.0092 (11)
C13	0.0217 (13)	0.0218 (13)	0.0219 (13)	0.0038 (10)	0.0016 (10)	−0.0016 (10)
C14	0.0106 (11)	0.0198 (12)	0.0143 (11)	−0.0008 (9)	0.0000 (9)	−0.0029 (9)
C15	0.0146 (11)	0.0134 (11)	0.0135 (11)	0.0019 (9)	0.0001 (9)	−0.0009 (9)
C16	0.0159 (12)	0.0155 (11)	0.0151 (11)	−0.0007 (9)	0.0017 (9)	0.0011 (9)
C17	0.0092 (11)	0.0186 (12)	0.0180 (12)	0.0010 (9)	−0.0001 (9)	−0.0025 (9)
C18	0.0171 (12)	0.0199 (12)	0.0144 (11)	0.0045 (10)	0.0000 (9)	0.0000 (9)
C19	0.0205 (12)	0.0151 (12)	0.0137 (11)	0.0008 (9)	0.0034 (10)	0.0034 (9)
C20	0.0151 (12)	0.0149 (11)	0.0153 (11)	0.0005 (9)	0.0044 (9)	−0.0030 (9)
C21	0.0147 (11)	0.0145 (11)	0.0142 (11)	−0.0008 (9)	0.0026 (9)	−0.0033 (9)
C22	0.0193 (12)	0.0147 (11)	0.0174 (12)	−0.0017 (10)	0.0051 (10)	−0.0026 (9)
C23	0.0176 (12)	0.0197 (12)	0.0235 (13)	−0.0062 (10)	0.0082 (10)	−0.0079 (10)
C24	0.0112 (11)	0.0242 (13)	0.0207 (12)	−0.0016 (10)	0.0007 (9)	−0.0119 (10)
C25	0.0143 (12)	0.0202 (12)	0.0159 (11)	0.0007 (10)	0.0004 (9)	−0.0055 (9)
C26	0.0135 (11)	0.0157 (11)	0.0142 (11)	0.0001 (9)	0.0039 (9)	−0.0061 (9)
Br3	0.01114 (12)	0.02792 (13)	0.02541 (13)	−0.00354 (10)	−0.00065 (9)	0.00470 (10)
Br4	0.01141 (12)	0.02510 (13)	0.02731 (13)	0.00130 (9)	0.00279 (9)	0.00374 (10)
O2	0.0185 (9)	0.0245 (9)	0.0200 (9)	−0.0008 (7)	0.0050 (7)	0.0069 (7)
C27	0.0087 (11)	0.0165 (11)	0.0126 (11)	−0.0010 (9)	0.0007 (9)	−0.0004 (9)
C28	0.0076 (11)	0.0178 (11)	0.0167 (12)	−0.0022 (9)	−0.0035 (9)	0.0023 (9)
C29	0.0099 (11)	0.0152 (11)	0.0210 (12)	−0.0023 (9)	−0.0034 (9)	0.0000 (9)
C30	0.0157 (12)	0.0189 (12)	0.0283 (14)	−0.0050 (10)	−0.0058 (10)	0.0048 (10)
C31	0.0228 (14)	0.0139 (12)	0.0398 (16)	−0.0013 (10)	−0.0087 (12)	−0.0017 (11)
C32	0.0240 (14)	0.0193 (13)	0.0356 (16)	0.0040 (11)	−0.0061 (12)	−0.0113 (11)
C33	0.0224 (13)	0.0241 (13)	0.0221 (13)	−0.0011 (11)	−0.0022 (10)	−0.0058 (10)
C34	0.0112 (11)	0.0187 (12)	0.0194 (12)	−0.0040 (9)	−0.0040 (9)	−0.0034 (10)
C35	0.0122 (11)	0.0194 (12)	0.0137 (11)	−0.0030 (9)	−0.0007 (9)	−0.0014 (9)
C36	0.0249 (14)	0.0274 (14)	0.0172 (12)	0.0001 (11)	0.0021 (10)	−0.0026 (10)
C37	0.0251 (14)	0.0362 (15)	0.0141 (12)	−0.0023 (12)	0.0006 (10)	0.0049 (11)
C38	0.0190 (13)	0.0239 (13)	0.0222 (13)	−0.0020 (10)	−0.0021 (10)	0.0095 (10)
C39	0.0152 (12)	0.0182 (12)	0.0186 (12)	−0.0009 (9)	−0.0006 (9)	0.0000 (9)
C40	0.0099 (11)	0.0185 (11)	0.0128 (11)	−0.0046 (9)	−0.0017 (9)	0.0005 (9)
C41	0.0143 (11)	0.0149 (11)	0.0116 (11)	−0.0027 (9)	−0.0013 (9)	0.0026 (9)
C42	0.0140 (11)	0.0173 (11)	0.0141 (11)	−0.0020 (9)	0.0024 (9)	0.0028 (9)
C43	0.0104 (11)	0.0230 (12)	0.0160 (11)	−0.0021 (9)	−0.0004 (9)	0.0062 (9)
C44	0.0181 (13)	0.0255 (13)	0.0169 (12)	−0.0078 (10)	−0.0015 (10)	−0.0001 (10)
C45	0.0197 (13)	0.0251 (13)	0.0175 (12)	−0.0044 (11)	0.0015 (10)	−0.0048 (10)

C46	0.0169 (12)	0.0173 (12)	0.0139 (11)	−0.0024 (10)	0.0014 (9)	0.0002 (9)
C47	0.0161 (12)	0.0167 (11)	0.0158 (11)	−0.0017 (9)	0.0010 (9)	0.0006 (9)
C48	0.0214 (13)	0.0212 (13)	0.0232 (13)	−0.0004 (10)	0.0029 (10)	−0.0070 (10)
C49	0.0175 (13)	0.0205 (13)	0.0262 (13)	0.0019 (10)	0.0067 (10)	−0.0026 (10)
C50	0.0108 (11)	0.0186 (12)	0.0219 (12)	0.0003 (9)	0.0018 (9)	0.0044 (10)
C51	0.0139 (11)	0.0172 (11)	0.0154 (11)	−0.0013 (9)	0.0003 (9)	0.0004 (9)
C52	0.0146 (11)	0.0135 (11)	0.0147 (11)	0.0013 (9)	0.0025 (9)	0.0026 (9)

Geometric parameters (Å, º)

Br1—C17	1.890 (2)	Br3—C43	1.901 (2)
Br2—C24	1.896 (2)	Br4—C50	1.908 (2)
O1—C2	1.219 (3)	O2—C28	1.216 (3)
C1—C15	1.520 (3)	C27—C40	1.523 (3)
C1—C14	1.529 (3)	C27—C52	1.524 (3)
C1—C26	1.536 (3)	C27—C28	1.541 (3)
C1—C2	1.541 (3)	C27—C41	1.544 (3)
C2—C3	1.475 (3)	C28—C29	1.476 (3)
C3—C4	1.407 (3)	C29—C34	1.404 (3)
C3—C8	1.407 (3)	C29—C30	1.405 (3)
C4—C5	1.381 (3)	C30—C31	1.383 (4)
C4—H4	0.9500	C30—H30	0.9500
C5—C6	1.384 (4)	C31—C32	1.385 (4)
C5—H5	0.9500	C31—H31	0.9500
C6—C7	1.387 (4)	C32—C33	1.385 (4)
C6—H6	0.9500	C32—H32	0.9500
C7—C8	1.402 (3)	C33—C34	1.401 (3)
C7—H7	0.9500	C33—H33	0.9500
C8—C9	1.480 (3)	C34—C35	1.485 (3)
C9—C14	1.395 (3)	C35—C40	1.403 (3)
C9—C10	1.409 (3)	C35—C36	1.407 (3)
C10—C11	1.377 (4)	C36—C37	1.382 (4)
C10—H10	0.9500	C36—H36	0.9500
C11—C12	1.381 (4)	C37—C38	1.385 (4)
C11—H11	0.9500	C37—H37	0.9500
C12—C13	1.390 (4)	C38—C39	1.386 (3)
C12—H12	0.9500	C38—H38	0.9500
C13—C14	1.396 (3)	C39—C40	1.396 (3)
C13—H13	0.9500	C39—H39	0.9500
C15—C16	1.376 (3)	C41—C42	1.384 (3)
C15—C20	1.400 (3)	C41—C46	1.403 (3)
C16—C17	1.394 (3)	C42—C43	1.401 (3)
C16—H16	0.9500	C42—H42	0.9500
C17—C18	1.393 (3)	C43—C44	1.388 (3)
C18—C19	1.386 (3)	C44—C45	1.391 (3)
C18—H18	0.9500	C44—H44	0.9500
C19—C20	1.395 (3)	C45—C46	1.391 (3)
C19—H19	0.9500	C45—H45	0.9500

C20—C21	1.464 (3)	C46—C47	1.463 (3)
C21—C22	1.392 (3)	C47—C48	1.390 (3)
C21—C26	1.405 (3)	C47—C52	1.404 (3)
C22—C23	1.387 (3)	C48—C49	1.388 (3)
C22—H22	0.9500	C48—H48	0.9500
C23—C24	1.389 (4)	C49—C50	1.386 (3)
C23—H23	0.9500	C49—H49	0.9500
C24—C25	1.392 (3)	C50—C51	1.392 (3)
C25—C26	1.385 (3)	C51—C52	1.385 (3)
C25—H25	0.9500	C51—H51	0.9500
C15—C1—C14	112.13 (18)	C40—C27—C52	113.59 (18)
C15—C1—C26	100.90 (18)	C40—C27—C28	114.62 (19)
C14—C1—C26	111.76 (18)	C52—C27—C28	110.03 (18)
C15—C1—C2	110.29 (18)	C40—C27—C41	112.67 (18)
C14—C1—C2	114.57 (19)	C52—C27—C41	100.86 (18)
C26—C1—C2	106.20 (18)	C28—C27—C41	103.81 (17)
O1—C2—C3	121.9 (2)	O2—C28—C29	122.2 (2)
O1—C2—C1	119.5 (2)	O2—C28—C27	119.5 (2)
C3—C2—C1	118.55 (19)	C29—C28—C27	118.16 (19)
C4—C3—C8	120.6 (2)	C34—C29—C30	120.9 (2)
C4—C3—C2	117.9 (2)	C34—C29—C28	121.2 (2)
C8—C3—C2	121.5 (2)	C30—C29—C28	117.9 (2)
C5—C4—C3	120.4 (2)	C31—C30—C29	120.0 (2)
C5—C4—H4	119.8	C31—C30—H30	120.0
C3—C4—H4	119.8	C29—C30—H30	120.0
C4—C5—C6	119.2 (2)	C30—C31—C32	119.6 (2)
C4—C5—H5	120.4	C30—C31—H31	120.2
C6—C5—H5	120.4	C32—C31—H31	120.2
C5—C6—C7	121.1 (2)	C33—C32—C31	120.7 (2)
C5—C6—H6	119.5	C33—C32—H32	119.6
C7—C6—H6	119.5	C31—C32—H32	119.6
C6—C7—C8	121.1 (2)	C32—C33—C34	121.1 (2)
C6—C7—H7	119.5	C32—C33—H33	119.4
C8—C7—H7	119.5	C34—C33—H33	119.4
C7—C8—C3	117.6 (2)	C33—C34—C29	117.6 (2)
C7—C8—C9	122.2 (2)	C33—C34—C35	121.7 (2)
C3—C8—C9	120.2 (2)	C29—C34—C35	120.6 (2)
C14—C9—C10	117.8 (2)	C40—C35—C36	118.2 (2)
C14—C9—C8	121.2 (2)	C40—C35—C34	120.5 (2)
C10—C9—C8	121.0 (2)	C36—C35—C34	121.3 (2)
C11—C10—C9	121.1 (2)	C37—C36—C35	121.4 (2)
C11—C10—H10	119.4	C37—C36—H36	119.3
C9—C10—H10	119.4	C35—C36—H36	119.3
C10—C11—C12	120.8 (2)	C36—C37—C38	119.8 (2)
C10—C11—H11	119.6	C36—C37—H37	120.1
C12—C11—H11	119.6	C38—C37—H37	120.1
C11—C12—C13	119.1 (2)	C37—C38—C39	119.9 (2)

C11—C12—H12	120.4	C37—C38—H38	120.1
C13—C12—H12	120.4	C39—C38—H38	120.1
C12—C13—C14	120.6 (2)	C38—C39—C40	120.8 (2)
C12—C13—H13	119.7	C38—C39—H39	119.6
C14—C13—H13	119.7	C40—C39—H39	119.6
C9—C14—C13	120.5 (2)	C39—C40—C35	119.9 (2)
C9—C14—C1	121.5 (2)	C39—C40—C27	119.0 (2)
C13—C14—C1	117.9 (2)	C35—C40—C27	121.1 (2)
C16—C15—C20	121.6 (2)	C42—C41—C46	121.5 (2)
C16—C15—C1	127.0 (2)	C42—C41—C27	128.0 (2)
C20—C15—C1	111.3 (2)	C46—C41—C27	110.35 (19)
C15—C16—C17	117.7 (2)	C41—C42—C43	117.0 (2)
C15—C16—H16	121.2	C41—C42—H42	121.5
C17—C16—H16	121.2	C43—C42—H42	121.5
C18—C17—C16	121.9 (2)	C44—C43—C42	122.6 (2)
C18—C17—Br1	120.57 (17)	C44—C43—Br3	118.75 (18)
C16—C17—Br1	117.56 (17)	C42—C43—Br3	118.68 (18)
C19—C18—C17	119.8 (2)	C43—C44—C45	119.4 (2)
C19—C18—H18	120.1	C43—C44—H44	120.3
C17—C18—H18	120.1	C45—C44—H44	120.3
C18—C19—C20	119.1 (2)	C46—C45—C44	119.4 (2)
C18—C19—H19	120.4	C46—C45—H45	120.3
C20—C19—H19	120.4	C44—C45—H45	120.3
C19—C20—C15	119.9 (2)	C45—C46—C41	120.1 (2)
C19—C20—C21	131.5 (2)	C45—C46—C47	130.9 (2)
C15—C20—C21	108.6 (2)	C41—C46—C47	109.0 (2)
C22—C21—C26	120.1 (2)	C48—C47—C52	120.5 (2)
C22—C21—C20	131.4 (2)	C48—C47—C46	131.1 (2)
C26—C21—C20	108.5 (2)	C52—C47—C46	108.5 (2)
C23—C22—C21	119.0 (2)	C49—C48—C47	118.9 (2)
C23—C22—H22	120.5	C49—C48—H48	120.5
C21—C22—H22	120.5	C47—C48—H48	120.5
C22—C23—C24	119.8 (2)	C50—C49—C48	119.7 (2)
C22—C23—H23	120.1	C50—C49—H49	120.2
C24—C23—H23	120.1	C48—C49—H49	120.2
C23—C24—C25	122.7 (2)	C49—C50—C51	122.7 (2)
C23—C24—Br2	118.51 (18)	C49—C50—Br4	118.06 (18)
C25—C24—Br2	118.82 (19)	C51—C50—Br4	119.25 (18)
C26—C25—C24	116.8 (2)	C52—C51—C50	117.2 (2)
C26—C25—H25	121.6	C52—C51—H51	121.4
C24—C25—H25	121.6	C50—C51—H51	121.4
C25—C26—C21	121.7 (2)	C51—C52—C47	121.1 (2)
C25—C26—C1	127.6 (2)	C51—C52—C27	127.6 (2)
C21—C26—C1	110.6 (2)	C47—C52—C27	111.3 (2)

Hydrogen-bond geometry (Å, º)

Cg2, Cg3, Cg6, Cg15 and Cg17 are the centroids of the C1–C3/C8/C9/C14, C3–C8, C21–C26, C29–C24 and C41–C46 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C44—H44···O1^{i}	0.95	2.44	3.364 (3)	163
C5—H5···*Cg*6^{ii}	0.95	2.69	3.554 (3)	151
C31—H31···*Cg*17^{iii}	0.95	2.88	3.780 (3)	158
C24—Br2···*Cg*15^{iv}	1.90 (1)	3.44 (1)	5.330 (3)	173 (1)
C50—Br4···*Cg*2	1.91 (1)	3.78 (1)	5.454 (3)	145 (1)
C50—Br4···*Cg*3	1.91 (1)	3.91 (1)	5.790 (3)	168 (1)

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