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(1*RS*,2*RS*,3*SR*,4*SR*,9*RS*)-1,2,3,9-Tetrabromo-1,2,3,4-tetrahydro-1,4-methanonaphthalene

Ísmail Çelik,[a] Cem Cüneyt Ersanlı,[b] Mehmet Akkurt,[c]* Arif Daştan[d] and Santiago García-Granda[e]

[a]Department of Physics, Faculty of Arts and Sciences, University of Cumhuriyet, 06532 Sivas, Turkey, [b]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey, [c]Department of Physics, Faculty of Arts and Sciences, University of Erciyes, 38039 Kayseri, Turkey, [d]Department of Chemistry, Faculty of Arts and Sciences, Atatürk University, 25240 Erzurum, Turkey, and [e]Departamento Química Física y Analítica, Facultad de Química, Universidad Oviedo, C/ Julián Clavería, 8, 33006 Oviedo (Asturias), Spain

Correspondence e-mail: akkurt@erciyes.edu.tr

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.035
wR factor = 0.089
Data-to-parameter ratio = 16.1

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

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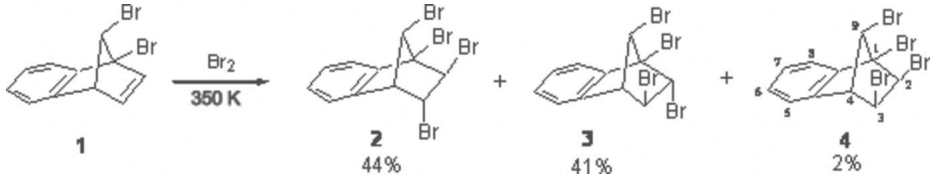
The title compound, $C_{11}H_8Br_4$, comprises a norbornane skeleton with four Br atoms, having a benzene ring fused on one side. The structure is stabilized by weak C—H···Br intramolecular hydrogen-bonding interactions in addition to van der Waals forces.

Comment

Polymeric materials and synthetic fibres are extensively used in many areas. The demand for non-burning or flame-retardant polymers is strong in various industries. Some of these flame retardant products contain brominated organic compounds (Burleigh *et al.*, 1980). Besides industrial applications for these highly brominated compounds, such as pesticides, plastics, fire-retardants and pharmaceutical chemicals, they also play an important role as key compounds for the synthesis of other derivatives (Altundaş *et al.*, 2002; Altundaş & Balcı, 1993). In this connection, great interest has been focused on the halogenation of benzonorbornadiene (Daştan *et al.*, 1994, 2002; Altundaş *et al.*, 2000; Cristol & Nachtigall, 1967). As a continuation of our interest in this area, the structure of tetrabromide (3), which was prepared by published methods (Daştan & Balcı, 2005) starting from 2,9-dibromobenzonorbornadiene, (1), by high-temperature bromination, is reported.



Compound (3) comprises a norbornane skeleton with four Br atoms, having a benzene ring fused on one side (Fig. 1). The average values of the Br—C bonds and the Br—C—C angles are 1.944 (3) Å and 114.7 (2)°, respectively (see Table 1). These values are within the ranges obtained for similar bonds in [1*R*(*S*),2*S*(*R*),3*S*(*R*),4*S*(*R*),9*R*(*S*)]-1,2,3,9-tetrabromo-1,2,3,4-tetrahydro-1,4-methanonaphthalene (Çelik *et al.*, 2006), which is one of a racemic pair of diastereomers with (3), and for those in similar compounds (Allen *et al.*, 1987; Çelik *et al.*, 2004; Akkurt *et al.*, 2004; Ersanlı *et al.*, 2005). The puckering parameters (Cremer & Pople, 1975) of the five-membered rings *A* (C1/C2/C5–C7) and *B* (C2–C5/C7) are Q_2 = 0.597 (4) Å and φ_2 = 70.93 (34)°, and Q_2 = 0.586 (3) Å and φ_2 = 132.31 (33)°, respectively. Ring *A* adopts an envelope conformation with atom C7 as the flap. However, owing to the repulsive interactions between the Br atoms in (3), ring *B*

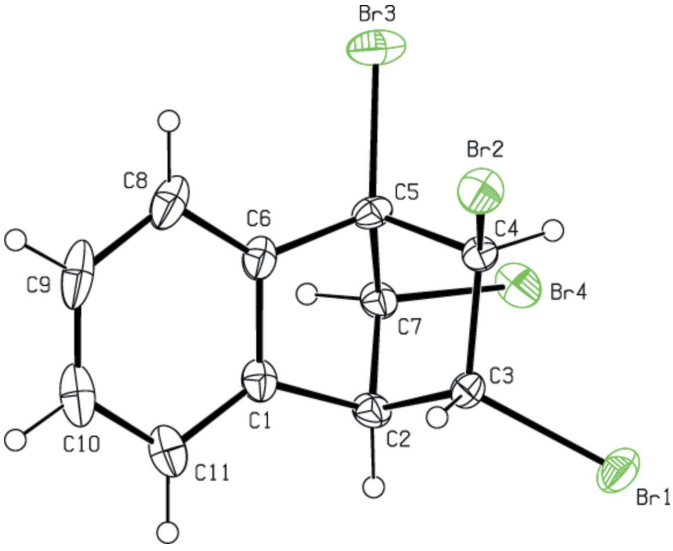


Figure 1
A view of (3), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

exhibits a conformation twisted about the C5—C7 bond. Plane *C* (C1/C2/C5/C6/C8–C11) has maximum deviations at C1, C2 and C9 of 0.020 (4), −0.017 (4) and −0.016 (5) Å, respectively. The dihedral angle between planes *D* (C2/C5/C7) and *C* is 56.64 (19)°, and that between planes *E* (C2–C5) [maximum deviation from planarity of 0.077 (4) Å for C2] and *C* is 68.69 (13)°, while that between planes *D* and *E* is 54.76 (22)° (Nardelli, 1999).

The crystal structure of (3) is stabilized by weak C—H···Br intramolecular hydrogen-bonding interactions in addition to van der Waals forces (Table 2).

Experimental

To a magnetically stirred solution of (1) (2.0 g, 6.67 mmol) (Daştan & Balcı, 2005) in refluxing CCl_4 (20 ml) was added dropwise a hot solution of bromine (1.52 g, 9.50 mmol) in CCl_4 (3 ml) over a period of 5 min. The resulting reaction mixture was heated for 1 min at reflux temperature. The solvent was evaporated, the residue was crystallized from CH_2Cl_2–*n*-pentane (1:2) and pure tetrabromide (3) was obtained (700 mg). After separation of the majority of (3), the residue was chromatographed on silica gel (100 g) using *n*-hexane as eluant. The first fraction was a mixture of tetrabromides (2) and (3). The solution was allowed to stand for 2 h in a refrigerator and the resulting crystals were identified as tetrabromide (2). After separation of the crystals, the residue was analysed by NMR. Tetrabromide (2) (Daştan & Balcı, 2005): 600 mg, crystals, 750 mg mixture, total 44% yield. Tetrabromide (3) (Daştan & Balcı, 2005): 700 mg, crystals, 555 mg mixture, total 41% yield. The second fraction (from a silica-gel column) was identified as tetrabromide (4) (Daştan & Balcı, 2005) (61 mg, 2% yield; m.p. 446–447 K). Spectroscopic analysis for (3): ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.51–7.24 (*m*, 4H, H-aryl), 5.12 (*d*, $J_{2,3}$ = 4.2 Hz, 1H, H2), 4.37 (*t*, $J_{4,9} = J_{3,9}$ = 1.9 Hz, 1H, H9), 3.80 (*m*, 2H, H3 and H4). Analysis calculated for $C_{11}H_8Br_4$: C 28.73, H 1.75%; found: C 28.34, H 1.66%. Crystals of (3) suitable for X-ray analysis were obtained by slow evaporation of a CH_2Cl_2–*n*-pentane (1:3) solution at room temperature.

Crystal data

$C_{11}H_8Br_4$	Z = 4
M_r = 459.77	D_x = 2.462 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 6.62230 (10) Å	μ = 12.94 mm^{-1}
b = 13.6489 (3) Å	T = 294 (2) K
c = 13.7353 (3) Å	Prism, colourless
β = 92.079 (1)°	0.13 × 0.10 × 0.09 mm
V = 1240.68 (4) Å^3	

Data collection

Nonius KappaCCD diffractometer	2200 measured reflections
φ and ω scans	2200 independent reflections
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	2163 reflections with $I > 2\sigma(I)$
T_{min} = 0.284, T_{max} = 0.389	θ_{max} = 25.3°
(expected range = 0.228–0.312)	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 1.8439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.089	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
S = 1.10	$\Delta\rho_{min}$ = −0.64 e Å^{-3}
2200 reflections	Extinction correction: *SHELXL97*
137 parameters	Extinction coefficient: 0.0193 (14)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Br1—C3	1.964 (3)	Br3—C5	1.917 (3)
Br2—C4	1.946 (3)	Br4—C7	1.949 (3)
Br1—C3—C2	114.23 (19)	Br3—C5—C6	116.8 (2)
Br1—C3—C4	112.8 (2)	Br3—C5—C7	116.2 (2)
Br2—C4—C3	112.9 (2)	Br4—C7—C2	116.8 (2)
Br2—C4—C5	113.08 (19)	Br4—C7—C5	115.5 (3)
Br3—C5—C4	113.6 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···Br4	0.98	2.79	3.199 (3)	106

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 and 0.98 Å for aromatic and methine H atoms, respectively, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *COLLECT* (Bruker, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

References

Akkurt, M., Çelik, İ., Erenler, R., Çakmak, O., Ersanlı, C. C. & Büyükgüngör, O. (2004). *Acta Cryst.* E**60**, o2096–o2098.

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Altundaş, A., Daştan, A., McKee, M. M. & Balcı, M. (2000). *Tetrahedron*, **56**, 6115–6120.
Altundaş, R. & Balcı, M. (1993). *Tetrahedron*, **49**, 6521–6526.
Altundaş, R., Daştan, A., Ünaldı, N. S., Güven, K., Uzun, O. & Balcı, M. (2002). *Eur. J. Org. Chem.* pp. 526–533.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2004). *COLLECT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burleigh, P. H., Nametz, R. C., Moore, P. O. & Jay, T. A. (1980). *J. Fire Retard. Chem.* **7**, 47–57.
Çelik, İ., Çakmak, O., Akkurt, M., Ersanlı, C. C. & Büyükgüngör, O. (2004). *Acta Cryst.* E**60**, o468–o470.
Çelik, İ., Ersanlı, C. C., Akkurt, M., Daştan, A. & García-Granda, S. (2006). *Acta Cryst.* E**62**. Submitted.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Cristol, S. J. & Nachtigall, G. W. (1967). *J. Org. Chem.* **32**, 3727–3737.
Daştan, A. & Balcı, M. (2005). *Tetrahedron*, **61**, 5481–5488.
Daştan, A., Demir, Ü. & Balcı, M. (1994). *J. Org. Chem.* **59**, 6534–6538.
Daştan, A., Uzundumlu, E. & Balcı, M. (2002). *Helv. Chim. Acta*, **81**, 2729–2739.
Ersanlı, C. C., Çoruh, U., Hökelek, T., Vázquez-López, E. M. & Daştan, A. (2005). *Acta Cryst.* E**61**, o263–o265.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Nardelli, M. (1999). *J. Appl. Cryst.* **32**, 563–571.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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(1*RS*,2*RS*,3*SR*,4*SR*,9*RS*)-1,2,3,9-Tetrabromo-1,2,3,4-tetrahydro-1,4-methanonaphthalene

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(1RS,2RS,3SR,4SR,9RS)-1,2,3,9-Tetrabromo-1,2,3,4-tetrahydro- 1,4-methanonaphthalene

Crystal data

$C_{11}H_8Br_4$
$M_r = 459.77$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.6220$ (1) Å
$b = 13.6490$ (3) Å
$c = 13.7350$ (3) Å
$\beta = 92.079$ (1)°
$V = 1240.60$ (4) Å^3
$Z = 4$
$F(000) = 856$
$D_x = 2.462$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2168 reflections
$\theta = 2.2$–$68.3°$
$\mu = 12.94$ mm^{-1}
$T = 294$ K
Prism, colourless
0.13 × 0.10 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
CCD scans
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
$T_{min} = 0.284$, $T_{max} = 0.389$
2200 measured reflections
2200 independent reflections
2163 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.1°$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 16$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.089$
$S = 1.10$
2200 reflections
137 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
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 1.8439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}
Extinction correction: SHELXL97, $fc^* = kfc[1+0.001xfc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0193 (14)

Special details

Experimental. 13 C NMR (50 MHz, CDCl3): δ 142.6, 142.0, 131.5, 130.6, 127.5, 122.7, 71,7, 62.8, 62.5, 56.3, 53.6. IR (KBr, cm-1): *v* 3055, 3030, 2979, 1447, 1421, 1396, 1294, 1268, 1242, 1165, 1140, 1012, 859.

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	0.92821 (7)	0.23070 (3)	0.53920 (3)	0.0464 (2)
Br2	0.92029 (7)	0.23801 (3)	0.84157 (3)	0.0421 (2)
Br3	0.43778 (7)	0.10350 (4)	0.83537 (3)	0.0525 (2)
Br4	0.43941 (6)	0.11631 (3)	0.57020 (3)	0.0411 (2)
C1	0.9261 (5)	−0.0217 (3)	0.7118 (3)	0.0317 (10)
C2	0.8455 (5)	0.0377 (3)	0.6273 (2)	0.0317 (10)
C3	0.9231 (6)	0.1422 (3)	0.6518 (2)	0.0302 (10)
C4	0.7788 (5)	0.1775 (2)	0.7304 (2)	0.0264 (9)
C5	0.6674 (5)	0.0822 (3)	0.7570 (2)	0.0287 (10)
C6	0.8192 (6)	0.0064 (2)	0.7932 (3)	0.0332 (10)
C7	0.6227 (5)	0.0394 (3)	0.6540 (2)	0.0298 (10)
C8	0.8600 (8)	−0.0332 (3)	0.8834 (3)	0.0475 (14)
C9	1.0176 (9)	−0.1020 (3)	0.8910 (4)	0.0571 (16)
C10	1.1242 (8)	−0.1294 (3)	0.8113 (4)	0.0536 (16)
C11	1.0815 (6)	−0.0902 (3)	0.7200 (3)	0.0428 (11)
H2	0.87420	0.01290	0.56230	0.0380*
H3	1.06000	0.13740	0.68100	0.0360*
H4	0.68170	0.22420	0.70140	0.0320*
H7	0.57190	−0.02780	0.65930	0.0360*
H8	0.78680	−0.01530	0.93720	0.0570*
H9	1.05070	−0.12970	0.95140	0.0690*
H10	1.22730	−0.17530	0.81900	0.0650*
H11	1.15380	−0.10890	0.66630	0.0510*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0546 (3)	0.0522 (3)	0.0328 (3)	−0.0001 (2)	0.0056 (2)	0.0137 (2)
Br2	0.0542 (3)	0.0390 (3)	0.0328 (3)	−0.0080 (2)	−0.0030 (2)	−0.0094 (2)
Br3	0.0512 (3)	0.0631 (3)	0.0446 (3)	−0.0122 (2)	0.0213 (2)	−0.0167 (2)
Br4	0.0396 (3)	0.0451 (3)	0.0380 (3)	0.0074 (2)	−0.0085 (2)	−0.0076 (2)
C1	0.0385 (19)	0.0258 (17)	0.0302 (18)	−0.0015 (13)	−0.0063 (14)	−0.0021 (14)
C2	0.0396 (19)	0.0331 (18)	0.0225 (17)	0.0074 (15)	0.0011 (14)	−0.0048 (14)
C3	0.0373 (18)	0.0319 (17)	0.0215 (16)	0.0039 (14)	0.0008 (13)	0.0044 (13)

C4	0.0304 (16)	0.0285 (16)	0.0200 (15)	0.0006 (13)	−0.0023 (13)	−0.0020 (12)
C5	0.0345 (17)	0.0338 (18)	0.0179 (15)	−0.0051 (14)	0.0029 (13)	−0.0049 (13)
C6	0.049 (2)	0.0246 (16)	0.0256 (17)	−0.0037 (15)	−0.0050 (15)	−0.0001 (13)
C7	0.0375 (18)	0.0282 (17)	0.0235 (16)	0.0030 (14)	−0.0021 (13)	−0.0052 (13)
C8	0.077 (3)	0.036 (2)	0.029 (2)	−0.016 (2)	−0.0063 (19)	0.0069 (16)
C9	0.086 (3)	0.033 (2)	0.050 (3)	−0.014 (2)	−0.031 (3)	0.0186 (19)
C10	0.068 (3)	0.029 (2)	0.062 (3)	0.0022 (19)	−0.023 (2)	0.0063 (19)
C11	0.046 (2)	0.0294 (19)	0.052 (2)	0.0030 (16)	−0.0105 (19)	−0.0019 (17)

Geometric parameters (Å, º)

Br1—C3	1.964 (3)	C6—C8	1.370 (6)
Br2—C4	1.946 (3)	C8—C9	1.405 (7)
Br3—C5	1.917 (3)	C9—C10	1.376 (8)
Br4—C7	1.949 (3)	C10—C11	1.383 (7)
C1—C2	1.498 (5)	C2—H2	0.9800
C1—C6	1.398 (6)	C3—H3	0.9800
C1—C11	1.392 (5)	C4—H4	0.9800
C2—C3	1.549 (6)	C7—H7	0.9800
C2—C7	1.533 (5)	C8—H8	0.9300
C3—C4	1.545 (5)	C9—H9	0.9300
C4—C5	1.546 (5)	C10—H10	0.9300
C5—C6	1.514 (5)	C11—H11	0.9300
C5—C7	1.549 (4)		
Br1···Br4	3.6326 (6)	Br4···H3^{v}	3.0000
Br1···Br4^{i}	3.7382 (6)	Br4···H2^{vii}	3.2300
Br1···Br3^{ii}	3.6022 (6)	Br4···H4	2.7900
Br2···Br3^{i}	3.8913 (7)	C3···Br4^{i}	3.654 (4)
Br2···Br3	3.6834 (7)	C6···H3	2.8800
Br2···Br4^{iii}	3.7151 (6)	C9···H4^{xi}	2.9800
Br3···Br1^{iv}	3.6022 (6)	C9···H8^{ix}	3.1000
Br3···Br2	3.6834 (7)	C10···H4^{xi}	2.8500
Br3···Br2^{v}	3.8913 (7)	H2···Br4^{vii}	3.2300
Br3···Br4	3.6467 (6)	H2···H2^{xii}	2.4600
Br4···C3^{v}	3.654 (4)	H3···Br4^{i}	3.0000
Br4···Br2^{vi}	3.7151 (6)	H3···C6	2.8800
Br4···Br1	3.6326 (6)	H4···Br4	2.7900
Br4···Br4^{vii}	3.8152 (6)	H4···C9^{x}	2.9800
Br4···Br1^{v}	3.7382 (6)	H4···C10^{x}	2.8500
Br4···Br3	3.6467 (6)	H7···Br2^{xi}	3.2000
Br1···H10^{viii}	3.2100	H8···Br3	3.1100
Br2···H9^{ix}	3.2000	H8···C9^{ix}	3.1000
Br2···H7^{x}	3.2000	H9···Br2^{ix}	3.2000
Br3···H8	3.1100	H10···Br1^{xiii}	3.2100
C2—C1—C6	107.1 (3)	C6—C8—C9	116.9 (4)
C2—C1—C11	131.9 (4)	C8—C9—C10	121.6 (5)

C6—C1—C11	120.9 (4)	C9—C10—C11	121.5 (4)
C1—C2—C3	102.9 (3)	C1—C11—C10	117.4 (4)
C1—C2—C7	98.2 (3)	C1—C2—H2	116.00
C3—C2—C7	104.4 (3)	C3—C2—H2	116.00
Br1—C3—C2	114.23 (19)	C7—C2—H2	116.00
Br1—C3—C4	112.8 (2)	Br1—C3—H3	109.00
C2—C3—C4	103.3 (3)	C2—C3—H3	109.00
Br2—C4—C3	112.9 (2)	C4—C3—H3	109.00
Br2—C4—C5	113.08 (19)	Br2—C4—H4	109.00
C3—C4—C5	102.4 (3)	C3—C4—H4	109.00
Br3—C5—C4	113.6 (2)	C5—C4—H4	109.00
Br3—C5—C6	116.8 (2)	Br4—C7—H7	110.00
Br3—C5—C7	116.2 (2)	C2—C7—H7	110.00
C4—C5—C6	109.6 (3)	C5—C7—H7	110.00
C4—C5—C7	100.3 (2)	C6—C8—H8	122.00
C6—C5—C7	98.3 (3)	C9—C8—H8	122.00
C1—C6—C5	105.9 (3)	C8—C9—H9	119.00
C1—C6—C8	121.7 (4)	C10—C9—H9	119.00
C5—C6—C8	132.4 (4)	C9—C10—H10	119.00
Br4—C7—C2	116.8 (2)	C11—C10—H10	119.00
Br4—C7—C5	115.5 (3)	C1—C11—H11	121.00
C2—C7—C5	94.0 (2)	C10—C11—H11	121.00

C6—C1—C2—C3	70.0 (3)	Br2—C4—C5—C6	−62.9 (3)
C6—C1—C2—C7	−36.9 (4)	Br2—C4—C5—C7	−165.7 (2)
C11—C1—C2—C3	−107.1 (5)	C3—C4—C5—Br3	−168.6 (2)
C11—C1—C2—C7	146.0 (4)	C3—C4—C5—C6	58.8 (3)
C2—C1—C6—C5	1.5 (4)	C3—C4—C5—C7	−43.9 (3)
C2—C1—C6—C8	−178.6 (4)	Br3—C5—C6—C1	159.1 (3)
C11—C1—C6—C5	178.9 (3)	Br3—C5—C6—C8	−20.8 (6)
C11—C1—C6—C8	−1.2 (6)	C4—C5—C6—C1	−70.0 (3)
C2—C1—C11—C10	177.2 (4)	C4—C5—C6—C8	110.1 (4)
C6—C1—C11—C10	0.4 (6)	C7—C5—C6—C1	34.1 (3)
C1—C2—C3—Br1	160.0 (2)	C7—C5—C6—C8	−145.8 (4)
C1—C2—C3—C4	−77.1 (3)	Br3—C5—C7—Br4	58.0 (3)
C7—C2—C3—Br1	−97.9 (3)	Br3—C5—C7—C2	−179.7 (3)
C7—C2—C3—C4	25.0 (3)	C4—C5—C7—Br4	−64.9 (3)
C1—C2—C7—Br4	176.4 (3)	C4—C5—C7—C2	57.5 (3)
C1—C2—C7—C5	55.2 (3)	C6—C5—C7—Br4	−176.7 (2)
C3—C2—C7—Br4	70.7 (3)	C6—C5—C7—C2	−54.4 (3)
C3—C2—C7—C5	−50.5 (3)	C1—C6—C8—C9	1.4 (6)
Br1—C3—C4—Br2	−102.6 (2)	C5—C6—C8—C9	−178.8 (4)
Br1—C3—C4—C5	135.5 (2)	C6—C8—C9—C10	−0.9 (7)
C2—C3—C4—Br2	133.6 (2)	C8—C9—C10—C11	0.2 (7)

C2—C3—C4—C5	11.7 (3)	C9—C10—C11—C1	0.0 (7)
Br2—C4—C5—Br3	69.7 (3)		

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) *x*−1/2, −*y*+1/2, *z*+1/2; (v) *x*−1, *y*, *z*; (vi) *x*−1/2, −*y*+1/2, *z*−1/2; (vii) −*x*+1, −*y*, −*z*+1; (viii) −*x*+5/2, *y*+1/2, −*z*+3/2; (ix) −*x*+2, −*y*, −*z*+2; (x) −*x*+3/2, *y*+1/2, −*z*+3/2; (xi) −*x*+3/2, *y*−1/2, −*z*+3/2; (xii) −*x*+2, −*y*, −*z*+1; (xiii) −*x*+5/2, *y*−1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Br4	0.98	2.79	3.199 (3)	106