Relative influence of noncovalent interactions on the melting points of a homologous series of 1,2-dibromo-4,5-dialkoxybenzenes

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organic compounds

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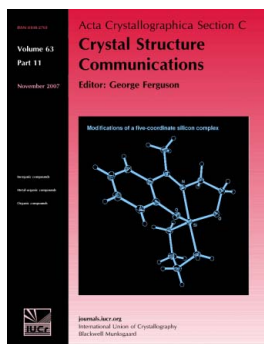
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Crystal structures are presented for two members of the homologous series of 1,2-dibromo-4,5-dialkoxybenzenes, *viz.* those with decyloxy and hexadecyloxy substituents, namely 1,2-dibromo-4,5-bis(decyloxy)benzene, $C_{26}H_{44}Br_2O_2$, (II), and 1,2-dibromo-4,5-bis(hexadecyloxy)benzene, $C_{38}H_{68}Br_2O_2$, (III). The relative influences which halogen bonding, π–π stacking and van der Waals interactions have on these structures are analysed and the results compared with those already found for the lightest homologue, 1,2-dibromo-4,5-dimethoxybenzene, (I) [Cukiernik, Zelcer, Garland & Baggio (2008). *Acta Cryst.* C**64**, o604–o608]. The results confirm that the prevalent interactions stabilizing the structures of (II) and (III) are van der Waals contacts between the aliphatic chains. In the case of (II), weak halogen C—Br···(Br—C)′ interactions are also present and contribute to the stability of the structure. In the case of (III), van der Waals interactions between the aliphatic chains are almost exclusive, weaker C—Br···π interactions being the only additional interactions detected. The results are in line with commonly accepted models concerning trends in crystal stability along a homologous series (as measured by their melting points), but the earlier report for $n = 1$, and the present report for $n = 10$ and 16, are among the few providing single-crystal information validating the hypothesis.

Comment

The design of advanced materials exhibiting selected crystalline structures based on specific intermolecular interactions is nowadays one of the main conceptual tools in materials science. Knowledge of the strength and directionality of noncovalent interactions (hydrogen bonds, π–π stacking,

halogen bonds *etc.*) allows for such design and hundreds of successful examples can be found in growing research fields like crystal engineering (Desiraju, 2003) or supramolecular chemistry (Steed & Atwood, 2009; Bruce, 2012). In most cases, the structure is governed by one prevalent interaction (and was designed on this basis). The predictability of the crystal structure that a given compound will adopt, on the basis of the intermolecular interactions it can exhibit, is high in such cases, but diminishes when the number of competing interactions rises. One way to explore the relative influence of different interactions, keeping some constant and allowing for a smooth variation of just one or two, is to work with different members of an homologous series.

In a study of the structure of dihalogenodimethoxybenzene compounds (Cukiernik *et al.*, 2008), we found that the structure of 1,2-dibromo-4,5-dimethoxybenzene, (I) (Scheme 1), extends through a combination of π–π, dipolar and halogen-bonding interactions. In this work, we report the crystal structures of two heavier homologues in this series, namely 1,2-dibromo-4,5-bis(decyloxy)benzene, (II), and 1,2-dibromo-4,5-bis(hexadecyloxy)benzene, (III), and analyse the relative influence halogen bonding, π–π stacking and van der Waals interactions have on the structures and, consequently, on some physical properties of these compounds.
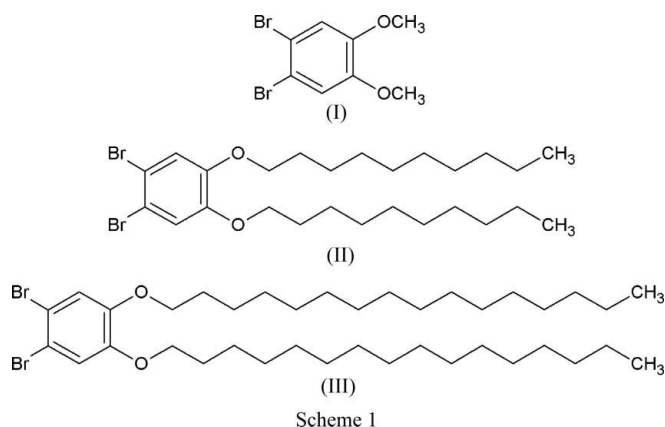
Scheme 1

Fig. 1 presents molecular views of both (II) and (III), where their striking 'jellyfish-like' geometry (which defines their packing characteristics) is apparent. The bond lengths and angles are unremarkable, and a distinguishing feature is the 'straight' character of the terminal aliphatic chains, as seen in the extremely narrow span of the C—C—C—C torsion angles, *i.e.* 171.0 (6)–179.9 (10)° in (II) and 174.13 (11)–179.9 (2)° in (III).

According to their geometric disposition, $C-X\cdots(X-C)'$ interactions (X = halogen) have historically been divided into types I and II (see Scheme 2); for further details, see Desiraju & Parthasarathy (1989, and references therein). In the case of (II) (Table 1) molecules interact weakly *via* C—Br···(Br—C)′ contacts of types I and II, some of them at the upper limit for stabilizing Br···Br distances. On the basis of accumulated experimental evidence, there is an increasing tendency to accept small (though not negligible) stabilization effects
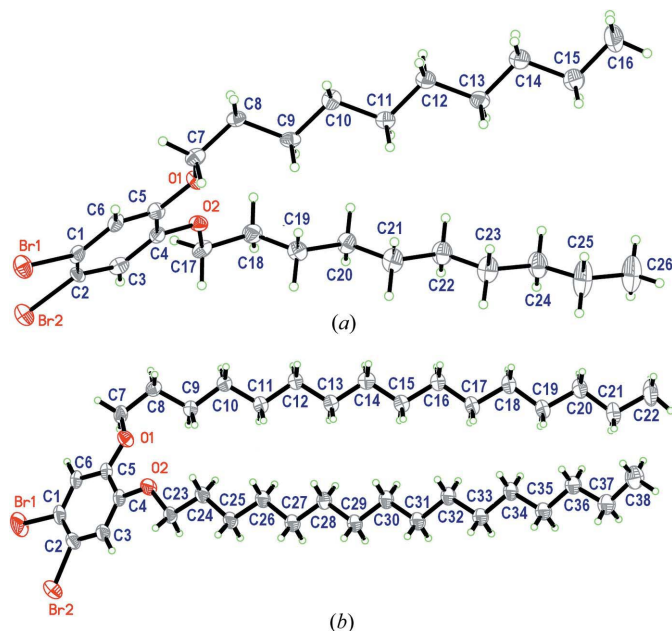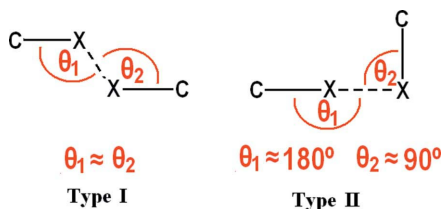
Figure 1
The molecular structutres of (*a*) (II) and (*b*) (III), showing the atom-numbering schemes. Displacement ellipsoids are drawn at the 40% probability level.

arising from rather long Br···Br contacts [up to 10% longer than twice the Br van der Waals radius, ~3.7 Å; see, for example, Jones & Kuś (2007, 2011) and Al-Far & Ali (2007)].

Scheme 2

The first and second entries, corresponding respectively to type I and type II contacts (Fig. 2*a*, labelled **A**), define dimeric units arranged in a head-to-head fashion (Fig. 2*a*, labelled **B**). In turn, as a consequence of a third C—Br···(Br—C)′ type-I contact (Table 1, entry 3) in conjunction with van der Waals interactions between aliphatic chains, these dimeric units are held together as one-dimensional strands parallel to *b*. van der Waals interactions between parallel aliphatic chains also link the dimeric units along *c*, defining broad planar arrays parallel to (100), ~*a*/2 wide along *a* (Fig. 2*a*, labelled **C**). Fig. 2(*b*) gives a simplified view of the way in which both kinds of Br···Br interactions build up.

The case of compound (III) is similar in general terms, *viz.* leading van der Waals interactions between aliphatic chains result in broad planar arrays parallel to (100), but the results are realized in quite different ways. To begin with, the head-to-head contacts joining antiparallel units in (II) are replaced by noticeably weaker C—Br···*π* contacts (Table 2) between parallel groups in (III), as shown in Fig. 3(*a*) (labelled **A**). These halogen···*π* interactions, presented in detail in Fig. 4, define columnar arrays along *c* (Fig. 3*b*, labelled **B**), which in
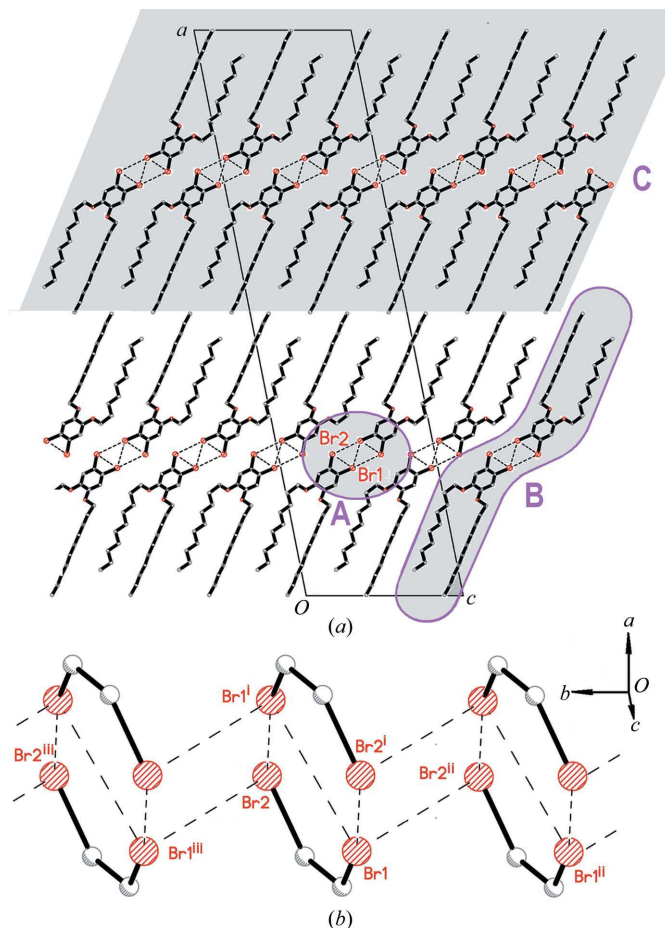
Figure 2
Packing diagrams for (II), depicting (*a*) a general view along *b* and (*b*) a simplified diagram showing halogen–halogen interactions. The areas labelled **A**, **B** and **C** are discussed in the *Comment*. [Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $x, y - 1, z$; (iii) $x, y + 1, z$.]

turn interleave their long aliphatic chains, linking them into broad planar arrays parallel to (100), ~*a*/2 wide along *a* (Fig. 3, labelled **C**).

These results are of significance for interpreting some physical properties of these compounds, namely their melting point (m.p.). Indeed, the trend of the m.p. along the whole homologous series, according to literature data (Sauer & Wegner, 1988; Kalashnikova *et al.*, 2003; Wöhrle & Schmidt, 1988; Hanack *et al.*, 1990), is shown in Fig. 5. In order to be able to discuss this trend in terms of the crystal structures solved here, we measured the m.p. of the structurally characterized compounds directly by differential scanning calorimetry (DSC) on single crystals from the same crop used for structure elucidation. Single crystals of (II) melt at 316.5 K (ΔH = 66 kJ mol^{-1}) and single crystals of (III) melt at 332.5 K (ΔH = 86 kJ mol^{-1}), very close to the previously reported values for powder samples. This agreement validates the use of the present structural information for the interpretation of the m.p. trend along the whole series.

This kind of behaviour (an initial decrease in m.p. with increasing chain length *n*, up to a certain value of *n*, then a progressive increase in m.p. with further increasing *n*, up to a
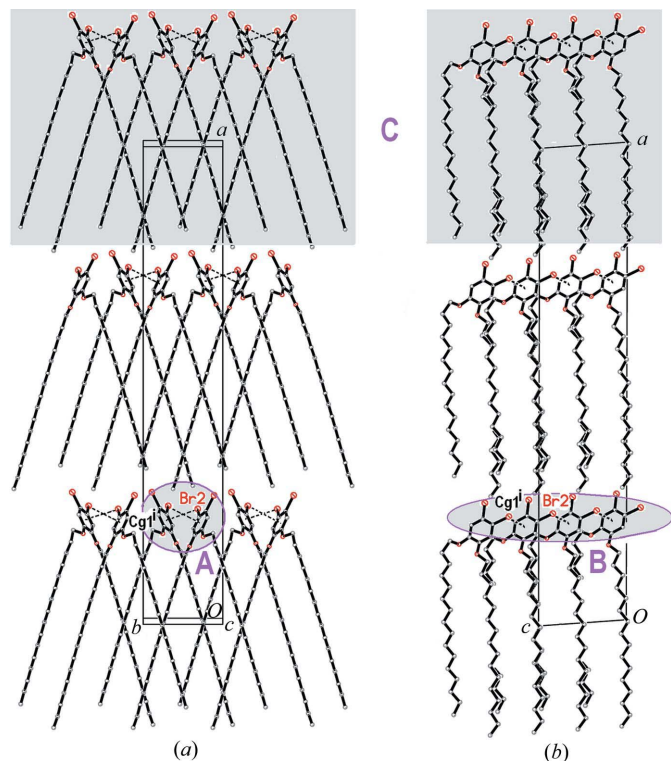
Figure 3
Packing diagrams for (III), depicting (a) a general view along c, showing the chains in projection, and (b) a general view along b, showing the chains running horizontally. The areas labelled **A**, **B** and **C** are discussed in the *Comment*. [Symmetry code: (i) $x, -y + 1, z - \frac{1}{2}$.]

limiting value) is frequently found in homologous series with polar components (aliphatic alcohols, aliphatic carboxylic acids *etc.*; Lutton, 1967; Weast, 1986) and is often interpreted in terms of a diblock molecular architecture, in which both molecular blocks (here denoted **1** and **2**) exhibit different packing requirements. For a homologous series, one of the molecular blocks (*e.g.* **2**) is the aliphatic chain; in such a case, the usual argument takes the form that, for short aliphatic chains, the packing is governed by the other block, **1**; increasing chain length progressively disturbs this packing,
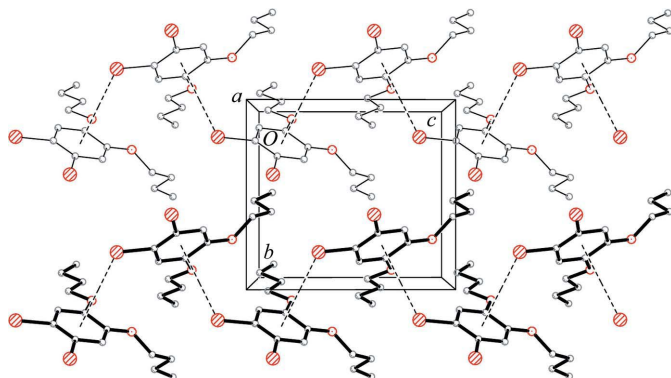
Figure 4
A packing view for (III), projected along c, showing a simplified version of the C—Br···π interactions. Terminal aliphatic tails have been shortened to a few C atoms, for clarity.
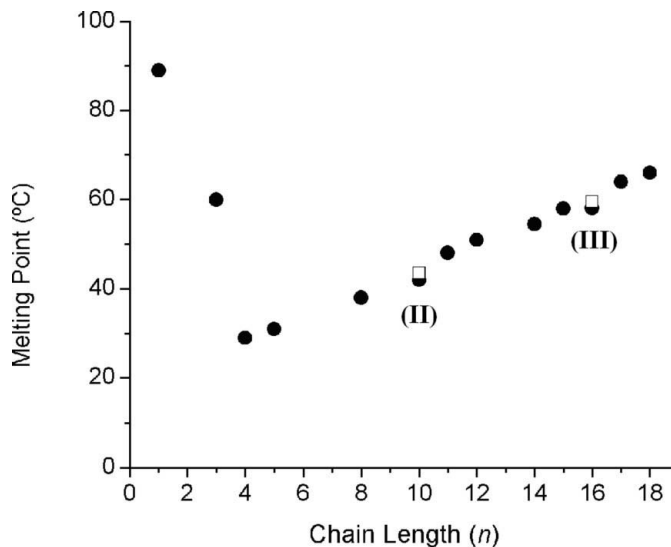
Figure 5
The melting points of 1,2-dibromo-4,5-dialkoxybenzenes as a function of alkoxy chain length. Filled circles represent literature data and open squares represent data for (II) and (III).

facilitating the melting process. For long-chain homologues, the packing of the aliphatic chains is the main driving force for the crystal structure; in those cases, block **1** acts as a disturbing agent for the packing, this effect being stronger (lower m.p.) as chain length decreases. These kinds of arguments are found in the fields of physical organic chemistry, polymers and liquid crystals (Platé Shibaev, 1974; Weber *et al.*, 1990; Ibn-Elhaj *et al.*, 1992). However, although these arguments are accepted and often based on powder X-ray diffraction evidence, they are not always supported by single-crystal crystallographic evidence.

In the present case, the structures of (I), (II) and (III) provide direct experimental support for this interpretation. Indeed, the crystal structure of (I) is essentially built up by π–π and halogen-bond interactions, while the prevalent interactions driving the structures of (II) and (III) are van der Waals interactions between the aliphatic chains. In the case of (II), halogen C—Br···(Br—C)′ contacts are still present and contribute to the overall stability of the structure. In the case of (III), van der Waals interactions between the aliphatic chains are almost exclusive, weaker C—Br···(ring centroid) contacts being the only additional interactions detected.

Possible future avenues for obtaining additional evidence for the homologous series under study could be to crystallize and solve the structure of the $n = 2$ homologue, as well as to find the 'transition point', *i.e.* the n value for which the head-to-head arrangement found in (II) is replaced by the 'tail-contact' arrangement found in (III). Further work on the subject is in progress.

Experimental

All chemical precursors were purchased from Aldrich and used without further purification. Differential scanning calorimetry (DSC)

Table 1
Geometry of the $C-X\cdots(X-C)'$ interactions (Å, °) in (II) (X = halogen).

The mean interaliphatic distance is 3.80 Å.

$C-X\cdots(X-C)'$	$X\cdots X'$	$(C-X)\cdots X'$	$X\cdots(X-C)'$	Interaction type
$C1-Br1\cdots(Br1-C1)^i$	3.7722 (15)	118.6 (2)	118.6 (2)	I
$C1-Br1\cdots(Br2-C2)^i$	3.6437 (10)	171.5 (2)	122.1 (2)	II
$C1-Br1\cdots(Br2-C2)^{ii}$	3.8704 (11)	73.0 (2)	91.0 (2)	I

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

Table 2
Geometry of the $C-X\cdots\pi$ interaction (Å, °) in (III) (X = halogen).

$Cg1$ is the centroid of the C1–C6 ring. The mean interaliphatic distance is 3.90 Å.

$C-X\cdots Cg$	$C-X$	$X\cdots Cg$	$C\cdots Cg$	$C-X\cdots Cg$
$C2-Br2\cdots Cg1^i$	1.893 (2)	3.976 (3)	4.941	109.1

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

was performed with a Shimadzu DSC-50 apparatus. Elemental analysis was carried out at the Servicio a Terceros of INQUIMAE on a Carlo Erba CHNS-O EA1108 analyser. ^{1}H NMR spectra were measured on a Bruker AM500 spectrometer, using CDCl$_3$ as solvent and its residual peaks as internal references (7.26 p.p.m. for ^{1}H).

Both (II) and (III) were synthesized in two steps from catechol (benzene-1,2-diol). The first step consisted of a Williamson's ether-ification of both hydroxy groups by reacting catechol with the appropriate bromoalkane, following published procedures (Boden *et al.*, 1993). The second step was an aromatic electrophilic substitution in the activated *para* positions relative to the alkoxy chains.

For the preparation of 1,2-dibromo-4,5-bis(decyloxy)benzene, (II), 1,2-bis(decyloxy)benzene (1.282 g) was dissolved in cold CH$_2$Cl$_2$ (16 ml), placed in a two-necked flask equipped with an NaHSO$_3$ bubbler with pressure compensation and immersed in an ice bath. Bromine (0.35 ml dissolved in 5 ml CH$_2$Cl$_2$) was added dropwise and the mixture was allowed to warm to room temperature. The progress of the reaction was monitored by thin-layer chromatography (TLC) (CH$_2$Cl$_2$–cyclohexane, 1:3 *v/v*). When the reaction was complete, it was stopped by the addition of aqueous NaHSO$_3$. The aqueous phase was discarded and the organic phase was washed successively with water, aqueous NaHSO$_3$ and water, and then dried with anhydrous Na$_2$SO$_4$, filtered and evaporated to dryness in a rotary evaporator. The solid was recrystallized from ethanol (yield 1.56 g, 87%). ^{1}H NMR (500 MHz, CD$_3$Cl): δ 7.058 (*s*, 2H), 3.94 (*t*, 4H), 1.78 (*q*, 4H), 1.44 (*q*, 4H), 1.34–1.27 (*m*, 24H), 0.88 (*t*, 6H). Single crystals were obtained by slow cooling (2 K per day) of a concentrated ethanol solution of (II).

For the preparation of 1,2-dibromo-4,5-bis(hexadecyloxy)benzene, (III), the synthetic procedure was identical to that followed for the preparation of (II), but using 1,2-bis(hexadecyloxy)benzene (2.009 g) dissolved in 25 ml CH$_2$Cl$_2$ instead of 1,2-bis(decyloxy)benzene and 0.40 ml Br$_2$ instead of 0.35 ml (yield 1.88 g, 73%). Analysis found (calculated for C$_{38}$H$_{68}$Br$_2$O$_2$) (%): C 63.6 (63.68), H 9.6 (9.56). ^{1}H NMR (500 MHz, CD$_3$Cl): δ 7.06 (*s*, 2H), 3.94 (*t*, 4H), 1.78 (*q*, 4H), 1.44 (*q*, 4H), 1.34–1.27 (*m*, 48H), 0.88 (*t*, 6H). Single crystals were obtained by slow cooling of and solvent evaporation from a concentrated solution of (III) in chloroform.

Compound (II)

Crystal data

C$_{26}$H$_{44}$Br$_2$O$_2$	$V = 5366.7$ (2) Å^3
$M_r = 548.43$	$Z = 8$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 67.0788$ (15) Å	$\mu = 3.04$ mm^{-1}
$b = 4.4717$ (1) Å	$T = 150$ K
$c = 18.2399$ (4) Å	$0.56 \times 0.27 \times 0.07$ mm
$\beta = 101.216$ (2)°	

Data collection

Oxford Gemini S Ultra CCD area-detector diffractometer	28792 measured reflections
	5387 independent reflections
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)	4981 reflections with $I > 2\sigma(I)$
$T_{min} = 0.42$, $T_{max} = 0.78$	$R_{int} = 0.068$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.069$	271 parameters
$wR(F^2) = 0.184$	H-atom parameters constrained
$S = 1.21$	$\Delta\rho_{max} = 1.67$ e Å^{-3}
5387 reflections	$\Delta\rho_{min} = -0.95$ e Å^{-3}

Compound (III)

Crystal data

C$_{38}$H$_{68}$Br$_2$O$_2$	$V = 3868$ (2) Å^3
$M_r = 716.72$	$Z = 4$
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 50.158$ (5) Å	$\mu = 2.13$ mm^{-1}
$b = 8.360$ (3) Å	$T = 294$ K
$c = 9.248$ (3) Å	$0.58 \times 0.32 \times 0.10$ mm
$\beta = 94.136$ (5)°	

Data collection

Oxford Gemini S Ultra CCD area-detector diffractometer	16641 measured reflections
	6905 independent reflections
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)	4926 reflections with $I > 2\sigma(I)$
$T_{min} = 0.45$, $T_{max} = 0.82$	$R_{int} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.053$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
$S = 0.84$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
6905 reflections	Absolute structure: Flack (1983), with 2716 Friedel pairs
379 parameters	Flack parameter: 0.087 (5)
2 restraints	

Compound (III) posed no problems, either in the data collection or in the model refinement. In contrast, (II) showed disorder in the hydrophilic region, for which a low-temperature data set was needed to resolve the problem. In this way, a reasonable model could be refined, even when neglecting some (impossible to model) disorder effects. This was evident in some important reflection outliers, as well as in some significant $\Delta\rho$ peaks, *e.g.* 1.67 e Å^{-3} at 2.04 Å from Br1.

All the H atoms in (III), and most of those in (II), were visible in difference maps, but they were subsequently placed in geometrically idealized positions and allowed to ride on their parent atoms, with aromatic C—H = 0.93 Å, methylene C—H = 0.97 Å and methyl

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C—H = 0.96 Å, and with $U_{iso}(H) = 1.2, 1.2$ and $1.5U_{eq}(C)$, respectively.

For both compounds, data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

References

Al-Far, R. & Ali, B. F. (2007). *Acta Cryst.* E**63**, m1701.
Boden, N., Borner, R. C., Bushby, R. J., Cammidge, A. N. & Jesudason, M. V. (1993). *Liq. Cryst.* **15**, 851–858.
Bruce, D. W. (2012). *Supramolecular Chemistry: From Molecules to Nanomaterials*, edited by P. A. Gale & J. W. Steed, pp. 3493–3514. London: John Wiley & Sons.
Cukiernik, F. D., Zelcer, A., Garland, M. T. & Baggio, R. (2008). *Acta Cryst.* C**64**, o604–o608.
Desiraju, G. R. (2003). *J. Mol. Struct.* **656**, 5–15.
Desiraju, G. R. & Parthasarathy, R. (1989). *J. Am. Chem. Soc.* **111**, 8725–8726.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hanack, M., Gül, A., Hirsch, A., Mandal, B. K., Subramanian, L. R. & Witke, E. (1990). *Mol. Cryst. Liq. Cryst.* **187**, 365–382.
Ibn-Elhaj, M., Guillon, D., Skoulios, A., Giroud-Godquin, A. M. & Maldivi, P. (1992). *Liq. Cryst.* **11**, 731–744.
Jones, P. G. & Kuś, P. (2007). *Z. Naturforsch. Teil B*, **62**, 725–731.
Jones, P. G. & Kuś, P. (2011). *Acta Cryst.* C**67**, o131–o133.
Kalashnikova, I. P., Zhukov, I. V., Tomilova, L. G. & Zefirova, N. S. (2003). *Russ. Chem. Bull.* **52**, 1709–1714.
Lutton, E. S. (1967). In *Fatty Acids*, edited by K. S. Markley. New York: Interscience Publishers.
Oxford Diffraction (2009). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.
Platé, N. A. & Shibaev, V. P. (1974). *J. Polym. Sci. Macromol. Rev.* **8**, 117–253.
Sauer, T. & Wegner, G. (1988). *Mol. Cryst. Liq. Cryst.* **162**, 97–118.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Steed, J. L. & Atwood, J. L. (2009). *Supramolecular Chemistry*, 2nd ed. London: John Wiley & Sons.
Weast, R. C. (1986). Editor. *Handbook of Chemistry and Physics*, 66th ed. Boca Raton: CRC Press.
Weber, P., Guillon, D., Skoulios, A. & Miller, R. D. (1990). *Liq. Cryst.* **8**, 825–837.
Wohrle, D. & Schmidt, V. (1988). *J. Chem. Soc. Dalton Trans.* pp. 549–551.

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(II) 1,2-Dibromo-4,5-bis(decyloxy)benzene

Crystal data

$C_{26}H_{44}Br_2O_2$	$F(000) = 2288$
$M_r = 548.43$	$D_x = 1.358$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Hall symbol: -C 2yc	Cell parameters from 11243 reflections
$a = 67.0788$ (15) Å	$\theta = 2.1$–25.8°
$b = 4.4717$ (1) Å	$\mu = 3.04$ mm^{-1}
$c = 18.2399$ (4) Å	$T = 150$ K
$\beta = 101.216$ (2)°	Plate, colourless
$V = 5366.7$ (2) Å^3	$0.56 \times 0.27 \times 0.07$ mm
$Z = 8$	

Data collection

Oxford Gemini S Ultra CCD area-detector diffractometer	28792 measured reflections
Radiation source: fine-focus sealed tube	5387 independent reflections
Graphite monochromator	4981 reflections with $I > 2\sigma(I)$
ω scans, thick slices	$R_{int} = 0.068$
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)	$\theta_{max} = 26.2°$, $\theta_{min} = 1.9°$
	$h = -82 \rightarrow 82$
	$k = -4 \rightarrow 5$
$T_{min} = 0.42$, $T_{max} = 0.78$	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.069$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.184$	
$S = 1.21$	H-atom parameters constrained
5387 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 122.7172P]$ where $P = (F_o^2 + 2F_c^2)/3$
271 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 1.67$ e Å^{-3}
	$\Delta\rho_{min} = -0.95$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
Br1	0.225869 (11)	0.04646 (19)	0.45773 (4)	0.0389 (2)
Br2	0.249896 (11)	0.45935 (19)	0.34532 (4)	0.0366 (2)
O1	0.17000 (7)	−0.1276 (11)	0.2145 (3)	0.0297 (10)
O2	0.18712 (7)	0.2238 (10)	0.1327 (2)	0.0276 (10)
C1	0.21452 (10)	0.1098 (16)	0.3549 (3)	0.0268 (14)
C2	0.22418 (8)	0.2811 (14)	0.3103 (3)	0.0220 (12)
C3	0.21497 (10)	0.3305 (15)	0.2353 (4)	0.0287 (14)
H3	0.2212	0.4568	0.2059	0.034*
C4	0.19705 (9)	0.1950 (15)	0.2051 (3)	0.0244 (13)
C5	0.18738 (9)	0.0024 (15)	0.2497 (4)	0.0268 (14)
C6	0.19618 (9)	−0.0303 (15)	0.3267 (4)	0.0265 (14)
H6	0.1897	−0.1443	0.3578	0.032*
C7	0.15963 (10)	−0.3154 (15)	0.2613 (4)	0.0300 (14)
H7A	0.1542	−0.1931	0.2968	0.036*
H7B	0.1691	−0.4591	0.2888	0.036*
C8	0.14293 (10)	−0.4722 (15)	0.2110 (4)	0.0271 (13)
H8A	0.1372	−0.6189	0.2401	0.033*
H8B	0.1486	−0.5802	0.1738	0.033*
C9	0.12568 (10)	−0.2721 (15)	0.1703 (4)	0.0279 (14)
H9A	0.1213	−0.1412	0.2065	0.034*
H9B	0.1309	−0.1473	0.1348	0.034*
C10	0.10730 (10)	−0.4473 (17)	0.1288 (4)	0.0317 (15)
H10A	0.1117	−0.5768	0.0924	0.038*
H10B	0.1022	−0.5737	0.1644	0.038*
C11	0.09000 (10)	−0.2517 (16)	0.0889 (4)	0.0302 (14)
H11A	0.0950	−0.1239	0.0536	0.036*
H11B	0.0854	−0.1240	0.1253	0.036*
C12	0.07198 (11)	−0.4314 (17)	0.0473 (5)	0.0373 (17)
H12A	0.0764	−0.5476	0.0084	0.045*
H12B	0.0677	−0.5705	0.0819	0.045*
C13	0.05388 (11)	−0.2398 (17)	0.0119 (4)	0.0341 (15)
H13A	0.0490	−0.1321	0.0511	0.041*
H13B	0.0584	−0.0933	−0.0206	0.041*
C14	0.03652 (11)	−0.4177 (19)	−0.0328 (5)	0.0409 (18)
H14A	0.0318	−0.5605	0.0000	0.049*
H14B	0.0415	−0.5296	−0.0711	0.049*
C15	0.01860 (12)	−0.223 (2)	−0.0699 (5)	0.049 (2)
H15A	0.0133	−0.1163	−0.0314	0.059*
H15B	0.0234	−0.0765	−0.1016	0.059*
C16	0.00144 (13)	−0.403 (3)	−0.1167 (6)	0.067 (3)

H16A	−0.0093	−0.2705	−0.1387	0.101*
H16B	−0.0036	−0.5456	−0.0855	0.101*
H16C	0.0065	−0.5067	−0.1556	0.101*
C17	0.19550 (10)	0.4289 (15)	0.0888 (4)	0.0280 (14)
H17A	0.2090	0.3645	0.0836	0.034*
H17B	0.1966	0.6247	0.1121	0.034*
C18	0.18131 (11)	0.4434 (18)	0.0114 (4)	0.0367 (16)
H18A	0.1875	0.5674	−0.0217	0.044*
H18B	0.1796	0.2440	−0.0099	0.044*
C19	0.16053 (11)	0.5708 (18)	0.0163 (4)	0.0341 (16)
H19A	0.1536	0.4312	0.0435	0.041*
H19B	0.1624	0.7562	0.0445	0.041*
C20	0.14738 (11)	0.6299 (18)	−0.0591 (4)	0.0343 (16)
H20A	0.1456	0.4440	−0.0870	0.041*
H20B	0.1544	0.7682	−0.0862	0.041*
C21	0.12653 (12)	0.758 (2)	−0.0558 (4)	0.0394 (18)
H21A	0.1283	0.9427	−0.0272	0.047*
H21B	0.1193	0.6185	−0.0297	0.047*
C22	0.11359 (12)	0.822 (2)	−0.1328 (4)	0.0416 (18)
H22A	0.1120	0.6397	−0.1620	0.050*
H22B	0.1205	0.9672	−0.1585	0.050*
C23	0.09249 (12)	0.944 (2)	−0.1275 (4)	0.045 (2)
H23A	0.0941	1.1203	−0.0960	0.055*
H23B	0.0853	0.7944	−0.1041	0.055*
C24	0.07956 (12)	1.026 (2)	−0.2054 (4)	0.047 (2)
H24A	0.0864	1.1828	−0.2278	0.057*
H24B	0.0785	0.8521	−0.2379	0.057*
C25	0.05857 (14)	1.129 (3)	−0.2000 (5)	0.075 (4)
H25A	0.0596	1.3030	−0.1677	0.090*
H25B	0.0518	0.9723	−0.1776	0.090*
C26	0.04596 (15)	1.209 (3)	−0.2762 (6)	0.076 (4)
H26A	0.0327	1.2735	−0.2705	0.114*
H26B	0.0447	1.0358	−0.3081	0.114*
H26C	0.0525	1.3664	−0.2982	0.114*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0387 (4)	0.0495 (5)	0.0265 (4)	−0.0037 (3)	0.0012 (3)	0.0035 (3)
Br2	0.0304 (4)	0.0450 (4)	0.0334 (4)	−0.0083 (3)	0.0035 (3)	−0.0020 (3)
O1	0.029 (2)	0.033 (3)	0.026 (2)	−0.006 (2)	0.0024 (18)	−0.001 (2)
O2	0.034 (2)	0.023 (2)	0.025 (2)	−0.0042 (19)	0.0049 (18)	0.0005 (19)
C1	0.035 (3)	0.029 (3)	0.014 (3)	0.010 (3)	−0.001 (2)	0.003 (3)
C2	0.014 (3)	0.025 (3)	0.027 (3)	−0.004 (2)	0.004 (2)	−0.008 (3)
C3	0.035 (3)	0.025 (3)	0.028 (3)	0.002 (3)	0.014 (3)	0.003 (3)
C4	0.028 (3)	0.023 (3)	0.021 (3)	0.005 (3)	0.004 (2)	0.000 (3)
C5	0.017 (3)	0.026 (3)	0.040 (4)	−0.003 (2)	0.011 (3)	−0.001 (3)
C6	0.022 (3)	0.024 (3)	0.035 (4)	0.003 (3)	0.009 (3)	0.008 (3)
C7	0.036 (3)	0.023 (3)	0.033 (3)	−0.001 (3)	0.013 (3)	0.009 (3)
C8	0.036 (3)	0.021 (3)	0.026 (3)	0.000 (3)	0.009 (3)	0.001 (3)

C9	0.031 (3)	0.022 (3)	0.035 (3)	−0.004 (3)	0.015 (3)	−0.004 (3)
C10	0.034 (3)	0.033 (4)	0.031 (3)	0.000 (3)	0.011 (3)	0.006 (3)
C11	0.035 (3)	0.027 (3)	0.029 (3)	−0.002 (3)	0.008 (3)	−0.001 (3)
C12	0.034 (4)	0.028 (4)	0.049 (4)	−0.004 (3)	0.006 (3)	−0.001 (3)
C13	0.039 (4)	0.032 (4)	0.030 (3)	0.000 (3)	0.004 (3)	−0.006 (3)
C14	0.039 (4)	0.036 (4)	0.047 (4)	−0.001 (3)	0.007 (3)	−0.003 (4)
C15	0.037 (4)	0.043 (5)	0.065 (6)	−0.001 (4)	0.005 (4)	−0.003 (4)
C16	0.038 (5)	0.068 (7)	0.085 (8)	−0.004 (5)	−0.013 (5)	0.006 (6)
C17	0.037 (3)	0.021 (3)	0.029 (3)	0.001 (3)	0.016 (3)	0.011 (3)
C18	0.039 (4)	0.035 (4)	0.035 (4)	0.001 (3)	0.006 (3)	0.001 (3)
C19	0.045 (4)	0.039 (4)	0.017 (3)	0.001 (3)	0.005 (3)	−0.003 (3)
C20	0.041 (4)	0.042 (4)	0.020 (3)	0.005 (3)	0.005 (3)	0.003 (3)
C21	0.049 (4)	0.056 (5)	0.016 (3)	0.006 (4)	0.011 (3)	0.005 (3)
C22	0.045 (4)	0.051 (5)	0.028 (4)	0.003 (4)	0.005 (3)	0.006 (4)
C23	0.044 (4)	0.064 (6)	0.030 (4)	0.007 (4)	0.012 (3)	0.008 (4)
C24	0.041 (4)	0.069 (6)	0.031 (4)	0.007 (4)	0.005 (3)	−0.001 (4)
C25	0.048 (5)	0.129 (11)	0.046 (5)	0.028 (6)	0.006 (4)	0.022 (7)
C26	0.050 (5)	0.125 (11)	0.051 (6)	0.024 (7)	0.002 (4)	0.018 (7)

Geometric parameters (Å, º)

Br1—C1	1.903 (6)	C14—H14B	0.9700
Br2—C2	1.895 (6)	C15—C16	1.523 (12)
O1—C5	1.348 (8)	C15—H15A	0.9700
O1—C7	1.465 (8)	C15—H15B	0.9700
O2—C4	1.365 (7)	C16—H16A	0.9600
O2—C17	1.405 (7)	C16—H16B	0.9600
C1—C2	1.369 (9)	C16—H16C	0.9600
C1—C6	1.387 (9)	C17—C18	1.543 (10)
C2—C3	1.406 (9)	C17—H17A	0.9700
C3—C4	1.363 (9)	C17—H17B	0.9700
C3—H3	0.9300	C18—C19	1.525 (10)
C4—C5	1.425 (9)	C18—H18A	0.9700
C5—C6	1.421 (9)	C18—H18B	0.9700
C6—H6	0.9300	C19—C20	1.506 (9)
C7—C8	1.479 (9)	C19—H19A	0.9700
C7—H7A	0.9700	C19—H19B	0.9700
C7—H7B	0.9700	C20—C21	1.524 (10)
C8—C9	1.535 (9)	C20—H20A	0.9700
C8—H8A	0.9700	C20—H20B	0.9700
C8—H8B	0.9700	C21—C22	1.528 (9)
C9—C10	1.531 (9)	C21—H21A	0.9700
C9—H9A	0.9700	C21—H21B	0.9700
C9—H9B	0.9700	C22—C23	1.536 (11)
C10—C11	1.521 (9)	C22—H22A	0.9700
C10—H10A	0.9700	C22—H22B	0.9700
C10—H10B	0.9700	C23—C24	1.558 (10)
C11—C12	1.525 (9)	C23—H23A	0.9700
C11—H11A	0.9700	C23—H23B	0.9700
C11—H11B	0.9700	C24—C25	1.504 (12)

C12—C13	1.522 (10)	C24—H24A	0.9700
C12—H12A	0.9700	C24—H24B	0.9700
C12—H12B	0.9700	C25—C26	1.522 (12)
C13—C14	1.511 (10)	C25—H25A	0.9700
C13—H13A	0.9700	C25—H25B	0.9700
C13—H13B	0.9700	C26—H26A	0.9600
C14—C15	1.530 (11)	C26—H26B	0.9600
C14—H14A	0.9700	C26—H26C	0.9600
C5—O1—C7	115.7 (5)	C14—C15—H15A	109.0
C4—O2—C17	116.1 (5)	C16—C15—H15B	109.0
C2—C1—C6	121.3 (6)	C14—C15—H15B	109.0
C2—C1—Br1	121.6 (5)	H15A—C15—H15B	107.8
C6—C1—Br1	117.0 (5)	C15—C16—H16A	109.5
C1—C2—C3	119.8 (6)	C15—C16—H16B	109.5
C1—C2—Br2	122.7 (5)	H16A—C16—H16B	109.5
C3—C2—Br2	117.5 (5)	C15—C16—H16C	109.5
C4—C3—C2	120.6 (6)	H16A—C16—H16C	109.5
C4—C3—H3	119.7	H16B—C16—H16C	109.5
C2—C3—H3	119.7	O2—C17—C18	107.8 (6)
C3—C4—O2	125.1 (6)	O2—C17—H17A	110.2
C3—C4—C5	120.1 (6)	C18—C17—H17A	110.2
O2—C4—C5	114.8 (6)	O2—C17—H17B	110.2
O1—C5—C6	125.5 (6)	C18—C17—H17B	110.2
O1—C5—C4	115.9 (6)	H17A—C17—H17B	108.5
C6—C5—C4	118.6 (6)	C19—C18—C17	111.7 (6)
C1—C6—C5	119.2 (6)	C19—C18—H18A	109.3
C1—C6—H6	120.4	C17—C18—H18A	109.3
C5—C6—H6	120.4	C19—C18—H18B	109.3
O1—C7—C8	107.4 (5)	C17—C18—H18B	109.3
O1—C7—H7A	110.2	H18A—C18—H18B	107.9
C8—C7—H7A	110.2	C20—C19—C18	113.0 (6)
O1—C7—H7B	110.2	C20—C19—H19A	109.0
C8—C7—H7B	110.2	C18—C19—H19A	109.0
H7A—C7—H7B	108.5	C20—C19—H19B	109.0
C7—C8—C9	115.6 (6)	C18—C19—H19B	109.0
C7—C8—H8A	108.4	H19A—C19—H19B	107.8
C9—C8—H8A	108.4	C19—C20—C21	114.1 (6)
C7—C8—H8B	108.4	C19—C20—H20A	108.7
C9—C8—H8B	108.4	C21—C20—H20A	108.7
H8A—C8—H8B	107.4	C19—C20—H20B	108.7
C10—C9—C8	113.5 (6)	C21—C20—H20B	108.7
C10—C9—H9A	108.9	H20A—C20—H20B	107.6
C8—C9—H9A	108.9	C20—C21—C22	113.3 (6)
C10—C9—H9B	108.9	C20—C21—H21A	108.9
C8—C9—H9B	108.9	C22—C21—H21A	108.9
H9A—C9—H9B	107.7	C20—C21—H21B	108.9
C11—C10—C9	114.1 (6)	C22—C21—H21B	108.9
C11—C10—H10A	108.7	H21A—C21—H21B	107.7

C9—C10—H10A	108.7	C21—C22—C23	112.0 (6)
C11—C10—H10B	108.7	C21—C22—H22A	109.2
C9—C10—H10B	108.7	C23—C22—H22A	109.2
H10A—C10—H10B	107.6	C21—C22—H22B	109.2
C10—C11—C12	113.1 (6)	C23—C22—H22B	109.2
C10—C11—H11A	109.0	H22A—C22—H22B	107.9
C12—C11—H11A	109.0	C22—C23—C24	112.5 (6)
C10—C11—H11B	109.0	C22—C23—H23A	109.1
C12—C11—H11B	109.0	C24—C23—H23A	109.1
H11A—C11—H11B	107.8	C22—C23—H23B	109.1
C13—C12—C11	113.8 (6)	C24—C23—H23B	109.1
C13—C12—H12A	108.8	H23A—C23—H23B	107.8
C11—C12—H12A	108.8	C25—C24—C23	112.0 (7)
C13—C12—H12B	108.8	C25—C24—H24A	109.2
C11—C12—H12B	108.8	C23—C24—H24A	109.2
H12A—C12—H12B	107.7	C25—C24—H24B	109.2
C14—C13—C12	113.6 (6)	C23—C24—H24B	109.2
C14—C13—H13A	108.9	H24A—C24—H24B	107.9
C12—C13—H13A	108.9	C24—C25—C26	111.9 (8)
C14—C13—H13B	108.9	C24—C25—H25A	109.2
C12—C13—H13B	108.9	C26—C25—H25A	109.2
H13A—C13—H13B	107.7	C24—C25—H25B	109.2
C13—C14—C15	113.4 (7)	C26—C25—H25B	109.2
C13—C14—H14A	108.9	H25A—C25—H25B	107.9
C15—C14—H14A	108.9	C25—C26—H26A	109.5
C13—C14—H14B	108.9	C25—C26—H26B	109.5
C15—C14—H14B	108.9	H26A—C26—H26B	109.5
H14A—C14—H14B	107.7	C25—C26—H26C	109.5
C16—C15—C14	113.0 (8)	H26A—C26—H26C	109.5
C16—C15—H15A	109.0	H26B—C26—H26C	109.5
C6—C1—C2—C3	3.4 (10)	C4—C5—C6—C1	−4.1 (9)
Br1—C1—C2—C3	−177.9 (5)	C5—O1—C7—C8	−171.5 (5)
C6—C1—C2—Br2	−176.7 (5)	O1—C7—C8—C9	−66.3 (7)
Br1—C1—C2—Br2	2.0 (8)	O2—C17—C18—C19	65.0 (8)
C1—C2—C3—C4	−3.9 (10)	C7—C8—C9—C10	−171.0 (6)
Br2—C2—C3—C4	176.1 (5)	C8—C9—C10—C11	179.4 (6)
C2—C3—C4—O2	−178.7 (6)	C9—C10—C11—C12	179.4 (6)
C2—C3—C4—C5	0.4 (10)	C10—C11—C12—C13	175.6 (6)
C17—O2—C4—C3	−5.4 (9)	C11—C12—C13—C14	176.9 (7)
C17—O2—C4—C5	175.5 (6)	C12—C13—C14—C15	−178.5 (7)
C7—O1—C5—C6	0.4 (9)	C13—C14—C15—C16	178.2 (8)
C7—O1—C5—C4	−177.5 (6)	C4—O2—C17—C18	−176.2 (5)
C3—C4—C5—O1	−178.3 (6)	C17—C18—C19—C20	171.6 (6)
O2—C4—C5—O1	0.8 (8)	C18—C19—C20—C21	−179.8 (7)
C3—C4—C5—C6	3.6 (9)	C19—C20—C21—C22	178.9 (7)
O2—C4—C5—C6	−177.2 (6)	C20—C21—C22—C23	178.5 (7)
C2—C1—C6—C5	0.7 (10)	C21—C22—C23—C24	177.0 (8)
Br1—C1—C6—C5	−178.1 (5)	C22—C23—C24—C25	177.0 (9)

| O1—C5—C6—C1 | 178.0 (6) | C23—C24—C25—C26 | −179.9 (10) |

(III) 1,2-Dibromo-4,5-bis(hexadecyloxy)benzene

Crystal data

$C_{38}H_{68}Br_2O_2$	$F(000) = 1528$
$M_r = 716.72$	$D_x = 1.231$ Mg m^{-3}
Monoclinic, Cc	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Hall symbol: C -2yc	Cell parameters from 8379 reflections
$a = 50.158$ (5) Å	$\theta = 3.6–29.0°$
$b = 8.360$ (3) Å	$\mu = 2.13$ mm^{-1}
$c = 9.248$ (3) Å	$T = 294$ K
$\beta = 94.136$ (5)°	Plate, colourless
$V = 3868$ (2) Å^3	$0.58 \times 0.32 \times 0.10$ mm
$Z = 4$	

Data collection

Oxford Gemini S Ultra CCD area-detector diffractometer	16641 measured reflections
	6905 independent reflections
Radiation source: fine-focus sealed tube	4926 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.024$
ω scans, thick slices	$\theta_{max} = 27.0°$, $\theta_{min} = 3.6°$
Absorption correction: multi-scan	$h = -55 \rightarrow 63$
(*CrysAlis PRO*; Oxford Diffraction, 2009)	$k = -10 \rightarrow 10$
$T_{min} = 0.45$, $T_{max} = 0.82$	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2]$
$S = 0.84$	where $P = (F_o^2 + 2F_c^2)/3$
6905 reflections	$(\Delta/\sigma)_{max} = 0.001$
379 parameters	$\Delta\rho_{max} = 0.26$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.17$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), **with how many Friedel pairs?**
Secondary atom site location: difference Fourier map	Flack parameter: 0.087 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Br1	0.265200 (6)	0.10931 (4)	0.61498 (3)	0.08034 (10)
Br2	0.233107 (6)	0.31448 (4)	0.34048 (2)	0.07120 (9)
O1	0.18247 (3)	0.24640 (17)	0.90673 (14)	0.0424 (3)
O2	0.15942 (3)	0.4158 (2)	0.70339 (15)	0.0475 (4)
C1	0.23212 (4)	0.2101 (3)	0.6346 (2)	0.0460 (5)

C2	0.21907 (4)	0.2945 (3)	0.5242 (2)	0.0437 (5)
C3	0.19459 (4)	0.3661 (3)	0.5428 (2)	0.0423 (5)
H3	0.1859	0.4242	0.4678	0.051*
C4	0.18326 (4)	0.3503 (2)	0.6741 (2)	0.0363 (5)
C5	0.19608 (4)	0.2611 (2)	0.7859 (2)	0.0359 (5)
C6	0.22054 (4)	0.1931 (3)	0.7672 (2)	0.0411 (5)
H6	0.2294	0.1359	0.8424	0.049*
C7	0.19065 (4)	0.1218 (3)	1.0097 (2)	0.0447 (5)
H7A	0.2063	0.1552	1.0697	0.054*
H7B	0.1949	0.0245	0.9592	0.054*
C8	0.16749 (4)	0.0940 (3)	1.1017 (2)	0.0439 (5)
H8A	0.1633	0.1932	1.1494	0.053*
H8B	0.1727	0.0162	1.1763	0.053*
C9	0.14270 (4)	0.0343 (3)	1.0145 (2)	0.0449 (5)
H9A	0.1475	−0.0583	0.9589	0.054*
H9B	0.1367	0.1169	0.9462	0.054*
C10	0.11952 (4)	−0.0115 (3)	1.1042 (2)	0.0458 (5)
H11A	0.1251	−0.0986	1.1687	0.055*
H11B	0.1152	0.0791	1.1637	0.055*
C11	0.09473 (5)	−0.0619 (3)	1.0130 (2)	0.0494 (6)
H10A	0.0992	−0.1534	0.9549	0.059*
H10B	0.0896	0.0246	0.9467	0.059*
C12	0.07085 (4)	−0.1052 (3)	1.0966 (2)	0.0489 (6)
H12A	0.0758	−0.1930	1.1616	0.059*
H12B	0.0664	−0.0143	1.1554	0.059*
C13	0.04641 (5)	−0.1527 (3)	1.0012 (3)	0.0513 (6)
H13A	0.0510	−0.2439	0.9430	0.062*
H13B	0.0417	−0.0651	0.9354	0.062*
C14	0.02199 (5)	−0.1954 (3)	1.0813 (2)	0.0507 (6)
H14A	0.0265	−0.2841	1.1462	0.061*
H14B	0.0174	−0.1048	1.1403	0.061*
C15	−0.00213 (5)	−0.2403 (3)	0.9834 (2)	0.0542 (6)
H15A	0.0026	−0.3307	0.9245	0.065*
H15B	−0.0064	−0.1516	0.9183	0.065*
C16	−0.02704 (5)	−0.2835 (3)	1.0589 (2)	0.0541 (6)
H16A	−0.0230	−0.3736	1.1228	0.065*
H16B	−0.0317	−0.1938	1.1186	0.065*
C17	−0.05075 (5)	−0.3254 (3)	0.9581 (3)	0.0568 (7)
H17A	−0.0460	−0.4148	0.8983	0.068*
H17B	−0.0548	−0.2352	0.8943	0.068*
C18	−0.07597 (5)	−0.3694 (3)	1.0318 (3)	0.0567 (6)
H18A	−0.0721	−0.4603	1.0949	0.068*
H18B	−0.0808	−0.2804	1.0919	0.068*
C19	−0.09948 (5)	−0.4099 (3)	0.9274 (3)	0.0599 (7)
H19A	−0.0946	−0.4989	0.8675	0.072*
H19B	−0.1032	−0.3190	0.8640	0.072*
C20	−0.12493 (5)	−0.4535 (3)	0.9980 (3)	0.0606 (7)
H20A	−0.1213	−0.5444	1.0615	0.073*
H20B	−0.1299	−0.3645	1.0576	0.073*

C21	−0.14827 (5)	−0.4942 (4)	0.8926 (3)	0.0752 (8)
H21A	−0.1433	−0.5831	0.8329	0.090*
H21B	−0.1520	−0.4032	0.8292	0.090*
C22	−0.17372 (6)	−0.5381 (5)	0.9634 (4)	0.0953 (10)
H22A	−0.1876	−0.5615	0.8897	0.143*
H22B	−0.1791	−0.4500	1.0214	0.143*
H22C	−0.1705	−0.6304	1.0239	0.143*
C23	0.14154 (4)	0.4670 (3)	0.5843 (2)	0.0419 (5)
H23A	0.1381	0.3803	0.5158	0.050*
H23B	0.1491	0.5562	0.5341	0.050*
C24	0.11629 (4)	0.5164 (3)	0.6499 (2)	0.0442 (5)
H24A	0.1202	0.6058	0.7148	0.053*
H24B	0.1102	0.4284	0.7074	0.053*
C25	0.09390 (4)	0.5642 (3)	0.5396 (2)	0.0451 (5)
H25A	0.0998	0.6536	0.4831	0.054*
H25B	0.0900	0.4755	0.4738	0.054*
C26	0.06862 (4)	0.6109 (3)	0.6091 (2)	0.0482 (6)
H26A	0.0726	0.7009	0.6732	0.058*
H26B	0.0633	0.5223	0.6683	0.058*
C27	0.04518 (5)	0.6556 (3)	0.5041 (2)	0.0495 (6)
H27A	0.0503	0.7454	0.4457	0.059*
H27B	0.0411	0.5662	0.4394	0.059*
C28	0.02041 (4)	0.6994 (3)	0.5790 (2)	0.0495 (6)
H28A	0.0246	0.7888	0.6434	0.059*
H28B	0.0156	0.6096	0.6384	0.059*
C29	−0.00362 (5)	0.7435 (3)	0.4789 (2)	0.0518 (6)
H29A	−0.0080	0.6546	0.4142	0.062*
H29B	0.0009	0.8342	0.4201	0.062*
C30	−0.02816 (4)	0.7856 (3)	0.5588 (2)	0.0522 (6)
H30A	−0.0325	0.6951	0.6186	0.063*
H30B	−0.0237	0.8748	0.6231	0.063*
C31	−0.05271 (5)	0.8290 (3)	0.4630 (3)	0.0535 (6)
H31A	−0.0574	0.7397	0.3991	0.064*
H31B	−0.0486	0.9196	0.4031	0.064*
C32	−0.07674 (4)	0.8709 (3)	0.5480 (2)	0.0545 (6)
H32A	−0.0806	0.7807	0.6091	0.065*
H32B	−0.0720	0.9607	0.6110	0.065*
C33	−0.10175 (5)	0.9127 (3)	0.4554 (2)	0.0542 (6)
H33A	−0.1066	0.8231	0.3923	0.065*
H33B	−0.0980	1.0033	0.3946	0.065*
C34	−0.12536 (5)	0.9535 (3)	0.5426 (3)	0.0562 (6)
H34A	−0.1289	0.8629	0.6039	0.067*
H34B	−0.1205	1.0431	0.6057	0.067*
C35	−0.15089 (5)	0.9956 (3)	0.4526 (3)	0.0573 (7)
H35A	−0.1560	0.9055	0.3907	0.069*
H35B	−0.1474	1.0855	0.3904	0.069*
C36	−0.17411 (5)	1.0383 (4)	0.5426 (3)	0.0585 (7)
H36A	−0.1771	0.9498	0.6072	0.070*
H36B	−0.1691	1.1305	0.6021	0.070*

C37	−0.19989 (5)	1.0751 (4)	0.4554 (3)	0.0706 (9)		
H37A	−0.2055	0.9813	0.3994	0.085*		
H37B	−0.1968	1.1606	0.3878	0.085*		
C38	−0.22209 (6)	1.1239 (4)	0.5483 (3)	0.0829 (9)		
H38A	−0.2381	1.1441	0.4875	0.124*		
H38B	−0.2170	1.2193	0.6011	0.124*		
H38C	−0.2253	1.0395	0.6152	0.124*		

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03922 (15)	0.1009 (2)	0.1034 (2)	0.02751 (17)	0.02233 (13)	0.0018 (2)
Br2	0.05548 (17)	0.1022 (2)	0.05902 (13)	0.00078 (17)	0.02555 (11)	−0.00573 (16)
O1	0.0394 (9)	0.0432 (8)	0.0460 (8)	0.0086 (7)	0.0122 (6)	0.0078 (7)
O2	0.0338 (9)	0.0651 (11)	0.0443 (8)	0.0207 (8)	0.0067 (6)	0.0098 (7)
C1	0.0251 (11)	0.0487 (15)	0.0649 (14)	0.0019 (10)	0.0069 (10)	−0.0076 (11)
C2	0.0369 (12)	0.0472 (14)	0.0488 (12)	−0.0037 (11)	0.0144 (10)	−0.0078 (10)
C3	0.0329 (13)	0.0474 (15)	0.0468 (12)	0.0016 (10)	0.0046 (9)	0.0010 (10)
C4	0.0234 (11)	0.0374 (13)	0.0480 (12)	0.0027 (9)	0.0029 (8)	−0.0030 (9)
C5	0.0263 (11)	0.0344 (11)	0.0470 (12)	−0.0037 (9)	0.0038 (9)	−0.0028 (9)
C6	0.0225 (11)	0.0460 (14)	0.0543 (12)	0.0021 (10)	−0.0007 (9)	−0.0010 (10)
C7	0.0286 (12)	0.0523 (15)	0.0523 (13)	0.0059 (11)	−0.0037 (10)	0.0133 (11)
C8	0.0394 (12)	0.0516 (14)	0.0397 (11)	0.0025 (11)	−0.0042 (9)	0.0122 (10)
C9	0.0354 (13)	0.0558 (14)	0.0432 (12)	−0.0045 (11)	0.0016 (9)	0.0021 (10)
C10	0.0399 (13)	0.0567 (15)	0.0409 (11)	−0.0069 (11)	0.0032 (9)	0.0032 (10)
C11	0.0399 (14)	0.0607 (16)	0.0483 (13)	−0.0076 (11)	0.0071 (10)	0.0016 (10)
C12	0.0372 (13)	0.0618 (15)	0.0481 (12)	−0.0042 (12)	0.0051 (10)	0.0010 (11)
C13	0.0393 (15)	0.0642 (16)	0.0512 (13)	−0.0077 (12)	0.0079 (10)	−0.0020 (11)
C14	0.0363 (13)	0.0621 (16)	0.0538 (13)	−0.0066 (12)	0.0037 (10)	0.0015 (12)
C15	0.0424 (15)	0.0686 (18)	0.0522 (13)	−0.0082 (12)	0.0084 (11)	0.0003 (11)
C16	0.0382 (14)	0.0708 (18)	0.0534 (13)	−0.0072 (12)	0.0045 (10)	0.0008 (12)
C17	0.0389 (15)	0.0754 (18)	0.0573 (14)	−0.0093 (13)	0.0110 (11)	0.0054 (12)
C18	0.0370 (14)	0.0742 (18)	0.0594 (14)	−0.0102 (12)	0.0074 (10)	0.0035 (12)
C19	0.0399 (14)	0.082 (2)	0.0582 (15)	−0.0121 (14)	0.0093 (11)	0.0050 (13)
C20	0.0395 (14)	0.0783 (18)	0.0646 (15)	−0.0063 (13)	0.0087 (11)	0.0055 (13)
C21	0.0376 (15)	0.105 (3)	0.0832 (19)	−0.0136 (16)	0.0081 (13)	0.0021 (16)
C22	0.0400 (18)	0.129 (3)	0.118 (3)	−0.0182 (19)	0.0089 (16)	0.008 (2)
C23	0.0280 (12)	0.0506 (14)	0.0474 (12)	0.0052 (10)	0.0050 (9)	0.0082 (10)
C24	0.0329 (12)	0.0549 (15)	0.0453 (12)	0.0069 (11)	0.0068 (9)	0.0058 (10)
C25	0.0312 (12)	0.0568 (15)	0.0482 (12)	0.0095 (11)	0.0081 (9)	0.0039 (10)
C26	0.0313 (12)	0.0657 (16)	0.0478 (12)	0.0115 (12)	0.0041 (9)	0.0027 (11)
C27	0.0341 (13)	0.0648 (16)	0.0502 (13)	0.0098 (12)	0.0061 (10)	0.0013 (11)
C28	0.0314 (12)	0.0655 (17)	0.0515 (12)	0.0112 (11)	0.0028 (9)	−0.0006 (11)
C29	0.0343 (13)	0.0702 (17)	0.0514 (13)	0.0092 (12)	0.0062 (10)	−0.0001 (11)
C30	0.0301 (12)	0.0715 (18)	0.0548 (13)	0.0124 (11)	0.0027 (9)	0.0017 (12)
C31	0.0357 (14)	0.0724 (18)	0.0528 (13)	0.0109 (12)	0.0063 (11)	0.0027 (12)
C32	0.0297 (12)	0.0799 (18)	0.0535 (13)	0.0136 (12)	0.0010 (10)	0.0025 (11)
C33	0.0378 (13)	0.0763 (19)	0.0488 (13)	0.0083 (12)	0.0043 (10)	0.0019 (12)
C34	0.0290 (13)	0.0838 (18)	0.0557 (14)	0.0123 (13)	0.0026 (10)	0.0023 (12)
C35	0.0388 (14)	0.083 (2)	0.0503 (13)	0.0137 (13)	0.0056 (10)	0.0026 (13)

C36	0.0384 (14)	0.0829 (19)	0.0542 (14)	0.0110 (13)	0.0026 (11)	−0.0015 (13)
C37	0.0430 (17)	0.101 (3)	0.0682 (18)	0.0147 (16)	0.0033 (13)	0.0016 (16)
C38	0.0439 (17)	0.112 (3)	0.092 (2)	0.0294 (17)	0.0051 (14)	−0.0060 (19)

Geometric parameters (Å, º)

Br1—C1	1.881 (2)	C20—H20B	0.9700
Br2—C2	1.893 (2)	C21—C22	1.521 (4)
O1—C5	1.357 (2)	C21—H21A	0.9700
O1—C7	1.451 (3)	C21—H21B	0.9700
O2—C4	1.360 (2)	C22—H22A	0.9600
O2—C23	1.435 (3)	C22—H22B	0.9600
C1—C2	1.369 (3)	C22—H22C	0.9600
C1—C6	1.401 (3)	C23—C24	1.501 (3)
C2—C3	1.388 (3)	C23—H23A	0.9700
C3—C4	1.383 (3)	C23—H23B	0.9700
C3—H3	0.9300	C24—C25	1.515 (3)
C4—C5	1.393 (3)	C24—H24A	0.9700
C5—C6	1.374 (3)	C24—H24B	0.9700
C6—H6	0.9300	C25—C26	1.514 (3)
C7—C8	1.506 (3)	C25—H25A	0.9700
C7—H7A	0.9700	C25—H25B	0.9700
C7—H7B	0.9700	C26—C27	1.516 (3)
C8—C9	1.517 (3)	C26—H26A	0.9700
C8—H8A	0.9700	C26—H26B	0.9700
C8—H8B	0.9700	C27—C28	1.510 (3)
C9—C10	1.525 (3)	C27—H27A	0.9700
C9—H9A	0.9700	C27—H27B	0.9700
C9—H9B	0.9700	C28—C29	1.511 (3)
C10—C11	1.512 (3)	C28—H28A	0.9700
C10—H11A	0.9700	C28—H28B	0.9700
C10—H11B	0.9700	C29—C30	1.522 (3)
C11—C12	1.515 (3)	C29—H29A	0.9700
C11—H10A	0.9700	C29—H29B	0.9700
C11—H10B	0.9700	C30—C31	1.508 (3)
C12—C13	1.511 (3)	C30—H30A	0.9700
C12—H12A	0.9700	C30—H30B	0.9700
C12—H12B	0.9700	C31—C32	1.526 (3)
C13—C14	1.519 (3)	C31—H31A	0.9700
C13—H13A	0.9700	C31—H31B	0.9700
C13—H13B	0.9700	C32—C33	1.508 (3)
C14—C15	1.506 (3)	C32—H32A	0.9700
C14—H14A	0.9700	C32—H32B	0.9700
C14—H14B	0.9700	C33—C34	1.519 (3)
C15—C16	1.518 (3)	C33—H33A	0.9700
C15—H15A	0.9700	C33—H33B	0.9700
C15—H15B	0.9700	C34—C35	1.518 (3)
C16—C17	1.499 (3)	C34—H34A	0.9700
C16—H16A	0.9700	C34—H34B	0.9700
C16—H16B	0.9700	C35—C36	1.522 (3)

C17—C18	1.524 (3)	C35—H35A	0.9700
C17—H17A	0.9700	C35—H35B	0.9700
C17—H17B	0.9700	C36—C37	1.505 (3)
C18—C19	1.508 (3)	C36—H36A	0.9700
C18—H18A	0.9700	C36—H36B	0.9700
C18—H18B	0.9700	C37—C38	1.511 (4)
C19—C20	1.519 (3)	C37—H37A	0.9700
C19—H19A	0.9700	C37—H37B	0.9700
C19—H19B	0.9700	C38—H38A	0.9600
C20—C21	1.507 (3)	C38—H38B	0.9600
C20—H20A	0.9700	C38—H38C	0.9600
C5—O1—C7	118.08 (16)	C22—C21—H21A	108.7
C4—O2—C23	118.49 (15)	C20—C21—H21B	108.7
C2—C1—C6	119.92 (19)	C22—C21—H21B	108.7
C2—C1—Br1	122.46 (16)	H21A—C21—H21B	107.6
C6—C1—Br1	117.60 (17)	C21—C22—H22A	109.5
C1—C2—C3	120.64 (19)	C21—C22—H22B	109.5
C1—C2—Br2	121.74 (16)	H22A—C22—H22B	109.5
C3—C2—Br2	117.60 (17)	C21—C22—H22C	109.5
C4—C3—C2	119.4 (2)	H22A—C22—H22C	109.5
C4—C3—H3	120.3	H22B—C22—H22C	109.5
C2—C3—H3	120.3	O2—C23—C24	105.69 (16)
O2—C4—C3	123.98 (19)	O2—C23—H23A	110.6
O2—C4—C5	115.67 (17)	C24—C23—H23A	110.6
C3—C4—C5	120.34 (19)	O2—C23—H23B	110.6
O1—C5—C6	124.96 (19)	C24—C23—H23B	110.6
O1—C5—C4	115.26 (18)	H23A—C23—H23B	108.7
C6—C5—C4	119.76 (19)	C23—C24—C25	113.97 (17)
C5—C6—C1	119.89 (19)	C23—C24—H24A	108.8
C5—C6—H6	120.1	C25—C24—H24A	108.8
C1—C6—H6	120.1	C23—C24—H24B	108.8
O1—C7—C8	106.76 (17)	C25—C24—H24B	108.8
O1—C7—H7A	110.4	H24A—C24—H24B	107.7
C8—C7—H7A	110.4	C26—C25—C24	112.64 (17)
O1—C7—H7B	110.4	C26—C25—H25A	109.1
C8—C7—H7B	110.4	C24—C25—H25A	109.1
H7A—C7—H7B	108.6	C26—C25—H25B	109.1
C7—C8—C9	112.76 (18)	C24—C25—H25B	109.1
C7—C8—H8A	109.0	H25A—C25—H25B	107.8
C9—C8—H8A	109.0	C25—C26—C27	115.21 (17)
C7—C8—H8B	109.0	C25—C26—H26A	108.5
C9—C8—H8B	109.0	C27—C26—H26A	108.5
H8A—C8—H8B	107.8	C25—C26—H26B	108.5
C8—C9—C10	114.92 (17)	C27—C26—H26B	108.5
C8—C9—H9A	108.5	H26A—C26—H26B	107.5
C10—C9—H9A	108.5	C28—C27—C26	113.06 (18)
C8—C9—H9B	108.5	C28—C27—H27A	109.0
C10—C9—H9B	108.5	C26—C27—H27A	109.0

H9A—C9—H9B	107.5	C28—C27—H27B	109.0
C11—C10—C9	113.27 (16)	C26—C27—H27B	109.0
C11—C10—H11A	108.9	H27A—C27—H27B	107.8
C9—C10—H11A	108.9	C27—C28—C29	115.14 (18)
C11—C10—H11B	108.9	C27—C28—H28A	108.5
C9—C10—H11B	108.9	C29—C28—H28A	108.5
H11A—C10—H11B	107.7	C27—C28—H28B	108.5
C10—C11—C12	115.50 (18)	C29—C28—H28B	108.5
C10—C11—H10A	108.4	H28A—C28—H28B	107.5
C12—C11—H10A	108.4	C28—C29—C30	113.36 (18)
C10—C11—H10B	108.4	C28—C29—H29A	108.9
C12—C11—H10B	108.4	C30—C29—H29A	108.9
H10A—C11—H10B	107.5	C28—C29—H29B	108.9
C13—C12—C11	113.76 (18)	C30—C29—H29B	108.9
C13—C12—H12A	108.8	H29A—C29—H29B	107.7
C11—C12—H12A	108.8	C31—C30—C29	115.16 (18)
C13—C12—H12B	108.8	C31—C30—H30A	108.5
C11—C12—H12B	108.8	C29—C30—H30A	108.5
H12A—C12—H12B	107.7	C31—C30—H30B	108.5
C12—C13—C14	115.21 (19)	C29—C30—H30B	108.5
C12—C13—H13A	108.5	H30A—C30—H30B	107.5
C14—C13—H13A	108.5	C30—C31—C32	113.24 (19)
C12—C13—H13B	108.5	C30—C31—H31A	108.9
C14—C13—H13B	108.5	C32—C31—H31A	108.9
H13A—C13—H13B	107.5	C30—C31—H31B	108.9
C15—C14—C13	113.97 (19)	C32—C31—H31B	108.9
C15—C14—H14A	108.8	H31A—C31—H31B	107.7
C13—C14—H14A	108.8	C33—C32—C31	114.63 (19)
C15—C14—H14B	108.8	C33—C32—H32A	108.6
C13—C14—H14B	108.8	C31—C32—H32A	108.6
H14A—C14—H14B	107.7	C33—C32—H32B	108.6
C14—C15—C16	115.77 (19)	C31—C32—H32B	108.6
C14—C15—H15A	108.3	H32A—C32—H32B	107.6
C16—C15—H15A	108.3	C32—C33—C34	113.54 (18)
C14—C15—H15B	108.3	C32—C33—H33A	108.9
C16—C15—H15B	108.3	C34—C33—H33A	108.9
H15A—C15—H15B	107.4	C32—C33—H33B	108.9
C17—C16—C15	114.32 (19)	C34—C33—H33B	108.9
C17—C16—H16A	108.7	H33A—C33—H33B	107.7
C15—C16—H16A	108.7	C35—C34—C33	114.82 (19)
C17—C16—H16B	108.7	C35—C34—H34A	108.6
C15—C16—H16B	108.7	C33—C34—H34A	108.6
H16A—C16—H16B	107.6	C35—C34—H34B	108.6
C16—C17—C18	115.2 (2)	C33—C34—H34B	108.6
C16—C17—H17A	108.5	H34A—C34—H34B	107.5
C18—C17—H17A	108.5	C34—C35—C36	113.76 (19)
C16—C17—H17B	108.5	C34—C35—H35A	108.8
C18—C17—H17B	108.5	C36—C35—H35A	108.8
H17A—C17—H17B	107.5	C34—C35—H35B	108.8

C19—C18—C17	113.8 (2)	C36—C35—H35B	108.8
C19—C18—H18A	108.8	H35A—C35—H35B	107.7
C17—C18—H18A	108.8	C37—C36—C35	114.6 (2)
C19—C18—H18B	108.8	C37—C36—H36A	108.6
C17—C18—H18B	108.8	C35—C36—H36A	108.6
H18A—C18—H18B	107.7	C37—C36—H36B	108.6
C18—C19—C20	114.9 (2)	C35—C36—H36B	108.6
C18—C19—H19A	108.5	H36A—C36—H36B	107.6
C20—C19—H19A	108.5	C36—C37—C38	113.0 (2)
C18—C19—H19B	108.5	C36—C37—H37A	109.0
C20—C19—H19B	108.5	C38—C37—H37A	109.0
H19A—C19—H19B	107.5	C36—C37—H37B	109.0
C21—C20—C19	114.5 (2)	C38—C37—H37B	109.0
C21—C20—H20A	108.6	H37A—C37—H37B	107.8
C19—C20—H20A	108.6	C37—C38—H38A	109.5
C21—C20—H20B	108.6	C37—C38—H38B	109.5
C19—C20—H20B	108.6	H38A—C38—H38B	109.5
H20A—C20—H20B	107.6	C37—C38—H38C	109.5
C20—C21—C22	114.4 (2)	H38A—C38—H38C	109.5
C20—C21—H21A	108.7	H38B—C38—H38C	109.5
C6—C1—C2—C3	1.1 (3)	C10—C11—C12—C13	179.2 (2)
Br1—C1—C2—C3	179.52 (16)	C11—C12—C13—C14	−179.4 (2)
C6—C1—C2—Br2	−177.56 (16)	C12—C13—C14—C15	179.3 (2)
Br1—C1—C2—Br2	0.9 (3)	C13—C14—C15—C16	−179.8 (2)
C1—C2—C3—C4	−0.6 (3)	C14—C15—C16—C17	179.2 (2)
Br2—C2—C3—C4	178.09 (16)	C15—C16—C17—C18	179.9 (2)
C23—O2—C4—C3	17.4 (3)	C16—C17—C18—C19	179.6 (2)
C23—O2—C4—C5	−161.66 (19)	C17—C18—C19—C20	−179.8 (2)
C2—C3—C4—O2	179.9 (2)	C18—C19—C20—C21	−179.9 (2)
C2—C3—C4—C5	−1.0 (3)	C19—C20—C21—C22	179.9 (3)
C7—O1—C5—C6	−15.4 (3)	C4—O2—C23—C24	174.14 (18)
C7—O1—C5—C4	163.21 (19)	O2—C23—C24—C25	−175.97 (19)
O2—C4—C5—O1	2.6 (3)	C23—C24—C25—C26	179.1 (2)
C3—C4—C5—O1	−176.50 (18)	C24—C25—C26—C27	−178.4 (2)
O2—C4—C5—C6	−178.69 (19)	C25—C26—C27—C28	179.4 (2)
C3—C4—C5—C6	2.2 (3)	C26—C27—C28—C29	−179.5 (2)
O1—C5—C6—C1	176.85 (19)	C27—C28—C29—C30	179.6 (2)
C4—C5—C6—C1	−1.7 (3)	C28—C29—C30—C31	−179.5 (2)
C2—C1—C6—C5	0.1 (3)	C29—C30—C31—C32	−179.7 (2)
Br1—C1—C6—C5	−178.44 (16)	C30—C31—C32—C33	−179.2 (2)
C5—O1—C7—C8	−160.79 (18)	C31—C32—C33—C34	179.9 (2)
O1—C7—C8—C9	62.6 (3)	C32—C33—C34—C35	−179.8 (2)
C7—C8—C9—C10	174.3 (2)	C33—C34—C35—C36	−179.2 (2)
C8—C9—C10—C11	176.9 (2)	C34—C35—C36—C37	−178.0 (3)
C9—C10—C11—C12	−178.7 (2)	C35—C36—C37—C38	−177.4 (3)

C—X···(X—C)′ interactions (Å, °) in (II) (X = halogen)

The mean interaliphatic distance is 3.80Å.

C—X···(X—C)′	X···X′	(C—X)···X′	X···(X—C)′	Interaction type
C1—Br1···(Br1-C1)[i]	3.7722 (15)	118.6 (2)	118.6 (2)	I
C1—Br1···(Br2-C2)[i]	3.6437 (10)	171.5 (2)	122.1 (2)	II
C1—Br1···(Br2-C2)[ii]	3.8704 (11)	73.0 (2)	91.0 (2)	I

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

C—X···π interactions (Å, °) in (III) (X = halogen)

Cg1 is the centre of the C1–C6 ring. The mean interaliphatic distance is 3.90 Å.

C—X···Cg	C···X	X···Cg	C···Cg	C—X···Cg
C2—Br2···Cg1[i]	1.893	3.976 (3)	4.941	109.1

Symmetry code: (i) x, -y + 1, z - 1/2.