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3,4-Bis(4-bromophenyl)-2,5-diphenylcyclopenta-2,4-dienone

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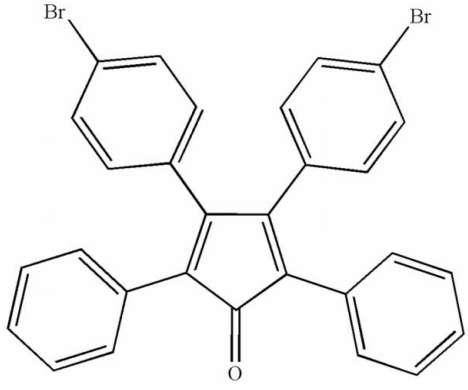
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.019; wR factor = 0.047; data-to-parameter ratio = 13.8.

The title compound, $C_{29}H_{18}Br_2O$, crystallizes as black–violet plates. The molecule displays a paddle-wheel conformation and the crystal packing is stabilized by C—H$\cdots\pi$ (C—H$\cdots\pi$ distances in the range 2.7–2.9 Å) and C—H$\cdots$Br contacts.

Related literature

The paddle-wheel conformation is also a typical feature of the parent substance tetraphenylcyclone (Barnes *et al.*, 1991; Alvarez-Toledano *et al.*, 1997) and the related compound phencyclone (Ruffani *et al.*, 2006), both involving C—H$\cdots\pi$ contacts in the crystal packing, similar to the title compound. For related literature, see: Dilthey *et al.* (1935).



Experimental

Crystal data

$C_{29}H_{18}Br_2O$
M_r = 542.25
Monoclinic, $P2_1/c$
a = 10.0677 (4) Å
b = 9.6526 (4) Å
c = 23.6791 (9) Å
β = 99.193 (2)°
V = 2271.57 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.59 mm^{-1}
T = 93 (2) K
0.20 × 0.19 × 0.18 mm

Data collection

Bruker KappaCCD APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.534, T_{max} = 0.564
(expected range = 0.496–0.524)
21955 measured reflections
3999 independent reflections
3578 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.047
S = 1.06
3999 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C28—H28$\cdots$Br1^{i}	0.95	2.87	3.6920 (18)	146
C22—H22$\cdots$Br2^{ii}	0.95	2.97	3.6386 (19)	129
C15—H15$\cdots$Br1^{iii}	0.95	3.03	3.8556 (18)	146

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2060).

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  doi:10.1107/S1600536807035702

supplementary materials

Acta Cryst. (2007). E**63**, o3966 [**doi:10.1107/S1600536807035702**]

3,4-Bis(4-bromophenyl)-2,5-diphenylcyclopenta-2,4-dienone

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Comment

The molecular geometry is best described by a paddle-wheel fashion, due to steric hindrance of the neighbouring aryl rings. The crystal packing is dominated by intramolecular C—H···π interactions. These intermolecular contacts, where π is an aromatic-ring centroid, with H···π distances ranging from 2.67 to 2.90 Å give rise to the formation of molecular chains extended along the *a* and *b* axis. Furthermore, unusual C—H···Br contacts forming a three-dimensional network can be observed (Figure 2).

Experimental

The title compound was synthesized according to the procedure described by Dilthey *et al.* (1935) from 1,2-bis(4-bromophenyl) ethane-1,2-dione, dibenzyl ketone and finely powdered potassium hydroxide in ethanol. Recrystallization from ethyl acetate yielded 72% dark-violet crystals.

Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å, and U_{iso} = 1.2–1.5 U_{eq}(parent atom).

Figures

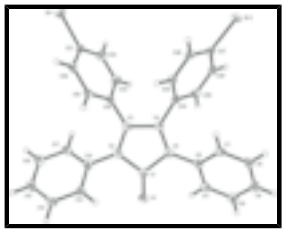

Fig. 1. Perspective view of (I), showing 50% probability displacement ellipsoids for the non-H atoms.

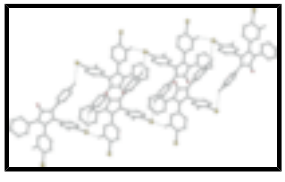

Fig. 2. Packing diagram of (I), viewed down the *b* axis, with C—H···Br contacts as broken lines.

3,4-Bis(4-bromophenyl)-2,5-diphenylcyclopenta-2,4-dienone

Crystal data

$C_{29}H_{18}Br_2O$ F_{000} = 1080

M_r = 542.25	D_x = 1.586 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.0677 (4) Å	Cell parameters from 5575 reflections
b = 9.6526 (4) Å	θ = 2.5–28.7º
c = 23.6791 (9) Å	μ = 3.59 mm^{-1}
β = 99.193 (2)º	T = 93 (2) K
V = 2271.57 (16) Å^3	Plate, dark-violet
Z = 4	0.20 × 0.19 × 0.18 mm

Data collection

Bruker KappaCCD APEXII area-detector diffractometer	3999 independent reflections
Radiation source: fine-focus sealed tube	3578 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 93(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −11→11
T_{min} = 0.534, T_{max} = 0.564	k = −11→11
21955 measured reflections	l = −23→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.019	H-atom parameters constrained
$wR(F^2)$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0196P)^2 + 1.357P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.002
3999 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
289 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.11380 (13)	0.81448 (14)	0.50405 (5)	0.0234 (3)
Br1	0.453140 (18)	0.255240 (19)	0.278725 (8)	0.02000 (6)
Br2	1.088680 (19)	0.50624 (2)	0.125864 (7)	0.02318 (6)
C1	1.06412 (18)	0.74769 (18)	0.46290 (7)	0.0171 (4)
C2	0.92780 (18)	0.67815 (18)	0.45385 (7)	0.0156 (4)
C3	0.91426 (18)	0.61459 (18)	0.40263 (7)	0.0152 (4)
C4	1.03677 (18)	0.64253 (18)	0.37486 (7)	0.0147 (4)
C5	1.12617 (18)	0.71972 (18)	0.40982 (7)	0.0155 (4)
C6	1.25237 (18)	0.78587 (18)	0.39981 (7)	0.0156 (4)
C7	1.26415 (19)	0.84047 (18)	0.34603 (8)	0.0173 (4)
H7	1.1912	0.8320	0.3154	0.021*
C8	1.38078 (19)	0.90662 (19)	0.33701 (8)	0.0203 (4)
H8	1.3872	0.9434	0.3003	0.024*
C9	1.48880 (19)	0.91968 (19)	0.38138 (8)	0.0220 (4)
H9	1.5690	0.9647	0.3750	0.026*
C10	1.47859 (19)	0.86662 (19)	0.43476 (8)	0.0217 (4)
H10	1.5521	0.8753	0.4651	0.026*
C11	1.36124 (19)	0.80057 (19)	0.44427 (8)	0.0187 (4)
H11	1.3550	0.7652	0.4812	0.022*
C12	0.83491 (18)	0.68419 (19)	0.49612 (7)	0.0154 (4)
C13	0.82388 (18)	0.80643 (19)	0.52658 (7)	0.0178 (4)
H13	0.8795	0.8833	0.5213	0.021*
C14	0.73240 (19)	0.8167 (2)	0.56443 (8)	0.0203 (4)
H14	0.7259	0.9002	0.5850	0.024*
C15	0.65065 (19)	0.7056 (2)	0.57225 (8)	0.0217 (4)
H15	0.5871	0.7133	0.5977	0.026*
C16	0.6614 (2)	0.5828 (2)	0.54287 (8)	0.0220 (4)
H16	0.6057	0.5062	0.5484	0.026*
C17	0.75368 (19)	0.57192 (19)	0.50535 (7)	0.0186 (4)
H17	0.7616	0.4872	0.4857	0.022*
C18	0.80114 (18)	0.52985 (18)	0.37389 (7)	0.0142 (4)
C19	0.66960 (18)	0.58029 (18)	0.36437 (7)	0.0162 (4)
H19	0.6517	0.6704	0.3774	0.019*
C20	0.56437 (18)	0.50109 (19)	0.33620 (8)	0.0173 (4)
H20	0.4751	0.5363	0.3296	0.021*
C21	0.59257 (18)	0.36977 (18)	0.31805 (7)	0.0153 (4)
C22	0.72124 (19)	0.31713 (19)	0.32679 (8)	0.0217 (4)
H22	0.7383	0.2267	0.3138	0.026*
C23	0.82536 (19)	0.39715 (19)	0.35460 (8)	0.0211 (4)
H23	0.9144	0.3614	0.3606	0.025*
C24	1.04490 (18)	0.59994 (18)	0.31555 (7)	0.0147 (4)
C25	0.94423 (18)	0.63988 (19)	0.27082 (7)	0.0173 (4)
H25	0.8671	0.6873	0.2793	0.021*
C26	0.95508 (18)	0.61145 (19)	0.21434 (8)	0.0183 (4)
H26	0.8871	0.6404	0.1841	0.022*

C27	1.06679 (19)	0.54023 (18)	0.20290 (7)	0.0166 (4)
C28	1.16667 (18)	0.49671 (18)	0.24641 (8)	0.0171 (4)
H28	1.2422	0.4469	0.2377	0.021*
C29	1.15549 (18)	0.52640 (18)	0.30265 (8)	0.0164 (4)
H29	1.2236	0.4965	0.3327	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0216 (7)	0.0311 (8)	0.0170 (7)	−0.0036 (6)	0.0015 (6)	−0.0078 (6)
Br1	0.01865 (11)	0.01994 (11)	0.02038 (10)	−0.00453 (8)	−0.00005 (7)	−0.00154 (7)
Br2	0.02779 (12)	0.02861 (11)	0.01347 (10)	−0.00723 (9)	0.00428 (8)	−0.00567 (8)
C1	0.0184 (10)	0.0169 (9)	0.0155 (9)	0.0032 (8)	0.0011 (8)	0.0006 (8)
C2	0.0164 (10)	0.0137 (9)	0.0162 (9)	0.0014 (8)	0.0011 (7)	0.0006 (7)
C3	0.0160 (10)	0.0143 (9)	0.0154 (9)	0.0033 (7)	0.0022 (7)	0.0019 (7)
C4	0.0150 (9)	0.0132 (9)	0.0155 (9)	0.0035 (7)	0.0013 (7)	0.0008 (7)
C5	0.0153 (9)	0.0164 (9)	0.0144 (9)	0.0035 (7)	0.0010 (7)	0.0017 (7)
C6	0.0151 (10)	0.0145 (9)	0.0174 (9)	0.0028 (7)	0.0029 (7)	−0.0028 (7)
C7	0.0199 (10)	0.0149 (9)	0.0169 (9)	0.0012 (8)	0.0023 (7)	−0.0028 (7)
C8	0.0268 (11)	0.0171 (9)	0.0187 (9)	0.0013 (8)	0.0091 (8)	−0.0024 (8)
C9	0.0176 (10)	0.0192 (10)	0.0311 (11)	−0.0013 (8)	0.0096 (8)	−0.0034 (8)
C10	0.0161 (10)	0.0218 (10)	0.0261 (10)	0.0027 (8)	−0.0001 (8)	−0.0042 (8)
C11	0.0198 (10)	0.0183 (9)	0.0180 (9)	0.0021 (8)	0.0030 (8)	0.0000 (7)
C12	0.0147 (9)	0.0197 (9)	0.0111 (8)	0.0032 (8)	−0.0006 (7)	0.0005 (7)
C13	0.0165 (10)	0.0193 (9)	0.0168 (9)	−0.0010 (8)	0.0002 (7)	−0.0007 (7)
C14	0.0212 (10)	0.0239 (10)	0.0148 (9)	0.0049 (8)	0.0003 (8)	−0.0040 (8)
C15	0.0201 (10)	0.0320 (11)	0.0138 (9)	0.0041 (9)	0.0052 (8)	0.0026 (8)
C16	0.0247 (11)	0.0247 (10)	0.0167 (9)	−0.0027 (9)	0.0039 (8)	0.0053 (8)
C17	0.0249 (11)	0.0167 (9)	0.0140 (9)	0.0025 (8)	0.0026 (8)	0.0008 (7)
C18	0.0168 (10)	0.0149 (9)	0.0114 (9)	−0.0007 (7)	0.0033 (7)	0.0011 (7)
C19	0.0200 (10)	0.0138 (9)	0.0155 (9)	0.0021 (8)	0.0049 (7)	−0.0012 (7)
C20	0.0142 (9)	0.0202 (10)	0.0180 (9)	0.0024 (8)	0.0037 (7)	0.0028 (7)
C21	0.0165 (10)	0.0165 (9)	0.0127 (9)	−0.0046 (8)	0.0013 (7)	0.0006 (7)
C22	0.0224 (11)	0.0154 (10)	0.0267 (10)	0.0025 (8)	0.0025 (8)	−0.0055 (8)
C23	0.0139 (10)	0.0204 (10)	0.0282 (11)	0.0042 (8)	0.0013 (8)	−0.0031 (8)
C24	0.0156 (9)	0.0133 (9)	0.0149 (9)	−0.0023 (7)	0.0018 (7)	−0.0008 (7)
C25	0.0157 (10)	0.0171 (9)	0.0192 (9)	0.0011 (8)	0.0029 (7)	−0.0004 (7)
C26	0.0168 (10)	0.0194 (10)	0.0169 (9)	−0.0025 (8)	−0.0027 (8)	0.0019 (7)
C27	0.0220 (10)	0.0147 (9)	0.0132 (9)	−0.0066 (8)	0.0036 (7)	−0.0025 (7)
C28	0.0164 (10)	0.0154 (9)	0.0205 (10)	−0.0004 (8)	0.0054 (8)	−0.0012 (7)
C29	0.0160 (10)	0.0159 (9)	0.0163 (9)	0.0001 (8)	−0.0010 (7)	0.0002 (7)

Geometric parameters (Å, °)

O1—C1	1.208 (2)	C14—C15	1.382 (3)
Br1—C21	1.9084 (17)	C14—H14	0.9500
Br2—C27	1.9006 (17)	C15—C16	1.387 (3)
C1—C2	1.512 (3)	C15—H15	0.9500
C1—C5	1.514 (2)	C16—C17	1.388 (3)

C2—C3	1.347 (2)	C16—H16	0.9500
C2—C12	1.476 (2)	C17—H17	0.9500
C3—C18	1.477 (2)	C18—C23	1.394 (3)
C3—C4	1.512 (2)	C18—C19	1.395 (3)
C4—C5	1.346 (3)	C19—C20	1.388 (3)
C4—C24	1.478 (2)	C19—H19	0.9500
C5—C6	1.475 (3)	C20—C21	1.382 (3)
C6—C11	1.400 (3)	C20—H20	0.9500
C6—C7	1.401 (2)	C21—C22	1.376 (3)
C7—C8	1.383 (3)	C22—C23	1.381 (3)
C7—H7	0.9500	C22—H22	0.9500
C8—C9	1.392 (3)	C23—H23	0.9500
C8—H8	0.9500	C24—C29	1.395 (3)
C9—C10	1.383 (3)	C24—C25	1.398 (2)
C9—H9	0.9500	C25—C26	1.386 (3)
C10—C11	1.392 (3)	C25—H25	0.9500
C10—H10	0.9500	C26—C27	1.381 (3)
C11—H11	0.9500	C26—H26	0.9500
C12—C17	1.396 (3)	C27—C28	1.385 (3)
C12—C13	1.397 (3)	C28—C29	1.384 (3)
C13—C14	1.388 (3)	C28—H28	0.9500
C13—H13	0.9500	C29—H29	0.9500
O1—C1—C2	126.91 (16)	C16—C15—H15	120.0
O1—C1—C5	126.30 (17)	C15—C16—C17	119.96 (18)
C2—C1—C5	106.78 (15)	C15—C16—H16	120.0
C3—C2—C12	130.15 (17)	C17—C16—H16	120.0
C3—C2—C1	106.79 (15)	C16—C17—C12	120.68 (17)
C12—C2—C1	123.06 (15)	C16—C17—H17	119.7
C2—C3—C18	128.82 (16)	C12—C17—H17	119.7
C2—C3—C4	109.77 (16)	C23—C18—C19	118.60 (16)
C18—C3—C4	121.41 (15)	C23—C18—C3	119.83 (16)
C5—C4—C24	127.24 (16)	C19—C18—C3	121.56 (16)
C5—C4—C3	110.06 (15)	C20—C19—C18	121.17 (16)
C24—C4—C3	122.44 (15)	C20—C19—H19	119.4
C4—C5—C6	130.49 (16)	C18—C19—H19	119.4
C4—C5—C1	106.56 (15)	C21—C20—C19	118.40 (17)
C6—C5—C1	122.44 (15)	C21—C20—H20	120.8
C11—C6—C7	118.40 (17)	C19—C20—H20	120.8
C11—C6—C5	120.93 (16)	C22—C21—C20	121.80 (17)
C7—C6—C5	120.62 (16)	C22—C21—Br1	117.45 (13)
C8—C7—C6	120.76 (17)	C20—C21—Br1	120.75 (14)
C8—C7—H7	119.6	C21—C22—C23	119.32 (17)
C6—C7—H7	119.6	C21—C22—H22	120.3
C7—C8—C9	120.38 (18)	C23—C22—H22	120.3
C7—C8—H8	119.8	C22—C23—C18	120.71 (17)
C9—C8—H8	119.8	C22—C23—H23	119.6
C10—C9—C8	119.55 (18)	C18—C23—H23	119.6
C10—C9—H9	120.2	C29—C24—C25	118.80 (16)
C8—C9—H9	120.2	C29—C24—C4	121.12 (16)

C9—C10—C11	120.43 (18)	C25—C24—C4	119.98 (16)
C9—C10—H10	119.8	C26—C25—C24	121.12 (17)
C11—C10—H10	119.8	C26—C25—H25	119.4
C10—C11—C6	120.49 (17)	C24—C25—H25	119.4
C10—C11—H11	119.8	C27—C26—C25	118.67 (17)
C6—C11—H11	119.8	C27—C26—H26	120.7
C17—C12—C13	118.57 (16)	C25—C26—H26	120.7
C17—C12—C2	121.74 (16)	C26—C27—C28	121.49 (16)
C13—C12—C2	119.66 (16)	C26—C27—Br2	119.80 (14)
C14—C13—C12	120.64 (17)	C28—C27—Br2	118.67 (14)
C14—C13—H13	119.7	C29—C28—C27	119.46 (17)
C12—C13—H13	119.7	C29—C28—H28	120.3
C15—C14—C13	120.14 (17)	C27—C28—H28	120.3
C15—C14—H14	119.9	C28—C29—C24	120.42 (17)
C13—C14—H14	119.9	C28—C29—H29	119.8
C14—C15—C16	119.99 (17)	C24—C29—H29	119.8
C14—C15—H15	120.0		
O1—C1—C2—C3	−179.45 (18)	C17—C12—C13—C14	−1.1 (3)
C5—C1—C2—C3	1.50 (19)	C2—C12—C13—C14	176.79 (17)
O1—C1—C2—C12	0.1 (3)	C12—C13—C14—C15	−0.2 (3)
C5—C1—C2—C12	−178.90 (15)	C13—C14—C15—C16	1.0 (3)
C12—C2—C3—C18	−0.8 (3)	C14—C15—C16—C17	−0.4 (3)
C1—C2—C3—C18	178.75 (17)	C15—C16—C17—C12	−0.9 (3)
C12—C2—C3—C4	178.56 (17)	C13—C12—C17—C16	1.7 (3)
C1—C2—C3—C4	−1.88 (19)	C2—C12—C17—C16	−176.19 (17)
C2—C3—C4—C5	1.7 (2)	C2—C3—C18—C23	−126.7 (2)
C18—C3—C4—C5	−178.89 (16)	C4—C3—C18—C23	54.0 (2)
C2—C3—C4—C24	−172.90 (16)	C2—C3—C18—C19	54.6 (3)
C18—C3—C4—C24	6.5 (2)	C4—C3—C18—C19	−124.71 (18)
C24—C4—C5—C6	1.8 (3)	C23—C18—C19—C20	−0.2 (3)
C3—C4—C5—C6	−172.48 (17)	C3—C18—C19—C20	178.54 (16)
C24—C4—C5—C1	173.62 (16)	C18—C19—C20—C21	0.5 (3)
C3—C4—C5—C1	−0.63 (19)	C19—C20—C21—C22	−0.5 (3)
O1—C1—C5—C4	−179.53 (18)	C19—C20—C21—Br1	−179.71 (13)
C2—C1—C5—C4	−0.47 (19)	C20—C21—C22—C23	0.2 (3)
O1—C1—C5—C6	−6.9 (3)	Br1—C21—C22—C23	179.40 (14)
C2—C1—C5—C6	172.18 (16)	C21—C22—C23—C18	0.2 (3)
C4—C5—C6—C11	−147.57 (19)	C19—C18—C23—C22	−0.2 (3)
C1—C5—C6—C11	41.7 (3)	C3—C18—C23—C22	−178.92 (17)
C4—C5—C6—C7	35.0 (3)	C5—C4—C24—C29	56.6 (3)
C1—C5—C6—C7	−135.76 (18)	C3—C4—C24—C29	−129.80 (18)
C11—C6—C7—C8	0.3 (3)	C5—C4—C24—C25	−119.9 (2)
C5—C6—C7—C8	177.85 (16)	C3—C4—C24—C25	53.7 (2)
C6—C7—C8—C9	0.2 (3)	C29—C24—C25—C26	−2.1 (3)
C7—C8—C9—C10	−0.3 (3)	C4—C24—C25—C26	174.47 (17)
C8—C9—C10—C11	0.0 (3)	C24—C25—C26—C27	1.1 (3)
C9—C10—C11—C6	0.5 (3)	C25—C26—C27—C28	0.3 (3)
C7—C6—C11—C10	−0.7 (3)	C25—C26—C27—Br2	−177.38 (13)
C5—C6—C11—C10	−178.20 (16)	C26—C27—C28—C29	−0.8 (3)

C3—C2—C12—C17	35.5 (3)	Br2—C27—C28—C29	176.94 (13)
C1—C2—C12—C17	−144.03 (18)	C27—C28—C29—C24	−0.2 (3)
C3—C2—C12—C13	−142.4 (2)	C25—C24—C29—C28	1.6 (3)
C1—C2—C12—C13	38.1 (2)	C4—C24—C29—C28	−174.91 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C28—H28···Br1^{i}	0.95	2.87	3.6920 (18)	146
C22—H22···Br2^{ii}	0.95	2.97	3.6386 (19)	129
C15—H15···Br1^{iii}	0.95	3.03	3.8556 (18)	146

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

Fig. 1

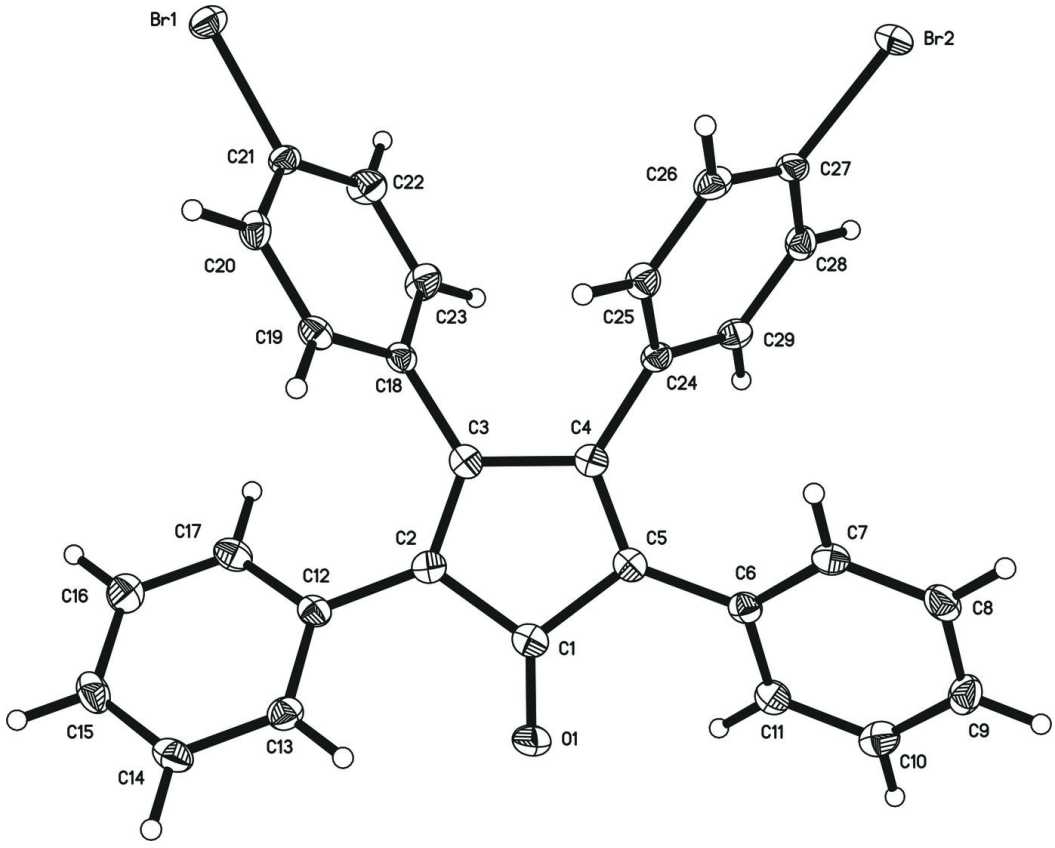
Br1
Br2
C21
C22
C26
C27
C20
C28
C23
C25
C19
C29
C18
C24
C3
C4
C17
C2
C5
C7
C12
C6
C16
C8
C1
C15
O1
C11
C9
C13
C10
C14

Fig. 2