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2,6-Bis[2-(4-benzyloxyphenyl)ethyl]-biphenyl

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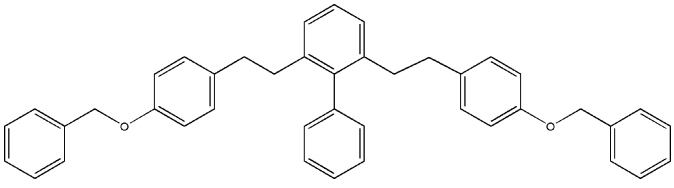
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.003 Å; R factor = 0.066; wR factor = 0.169; data-to-parameter ratio = 18.5.

The title compound, $C_{42}H_{38}O_2$, comprises a biphenyl system linked symmetrically at the 2- and 6-positions *via* two ethanediyl chains to two benzyloxyphenyl units. Both the ethanediyl and the benzyl ether linkages in the molecule are *trans* in the solid state, reinforcing the probability of a re-entrant structure. The rings of the biphenyl are inclined at 85.34 (8)° to one another. In the crystal structure, molecules form centrosymmetric dimers through C—H···O hydrogen bonds and are further linked into a three-dimensional network by a series of C—H···π interactions.

Related literature

For information on auxetic materials, see: Evans *et al.* (1991); Aldred & Moratti (2005). No structures of benzyloxy ethylbenzene derivatives of biphenyl have been reported previously but two molecules with linked benzyloxybenzene systems are known; see Roesky *et al.* (1997); Cannon *et al.* (1989).



Experimental

Crystal data

$C_{42}H_{38}O_2$
M_r = 574.72
Triclinic, $P\overline{1}$
a = 10.0431 (3) Å
b = 10.2145 (3) Å
c = 16.4136 (5) Å
α = 100.213 (2)°
β = 98.218 (2)°
γ = 98.642 (2)°
V = 1613.22 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 180 (2) K
0.30 × 0.18 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.971, T_{max} = 0.980
22105 measured reflections
7345 independent reflections
5114 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.169
S = 1.02
7345 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

*Cg*1, *Cg*3 and *Cg*5 are the centroids of the C1–C6, C17–C22 and C31–C36 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···O8^{i}	0.95	2.48	3.326 (4)	149
C2—H2A···*Cg*5^{ii}	0.95	2.78	3.644 (2)	152
C7—H7B···*Cg*1^{iii}	0.99	2.68	3.575 (3)	150
C13—H13A···*Cg*1^{iv}	0.95	2.82	3.620 (2)	143
C28—H28A···*Cg*3^{v}	0.95	2.98	3.865 (2)	155

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x, y, z+1$; (iii) $-x, -y, -z+2$; (iv) $-x, -y+1, -z+2$; (v) $-x+1, -y+1, -z+1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *enCIFer* (Allen *et al.*, 2004) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2317).

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supplementary materials

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2,6-Bis[2-(4-benzyloxyphenyl)ethyl]biphenyl

S. C. Moratti, J. Simpson and S. M. Tierney

Comment

Auxetic materials are those with a negative Poisson ratio, *i.e.* they expand sideways upon stretching (Evans *et al.*, 1991). A common theme in auxetic materials is that of the re-entrant structural motif. In this way, any force along one axis gets transmitted in a lateral fashion to a perpendicular axis. We were interested to see if such a unit could be deliberately designed into a polymer backbone. Computer simulations of such structures suggest that, under ideal situations, the resulting material should be auxetic (Evans *et al.*, 1991; Aldred & Moratti, 2005). While rigid auxetic molecular structures are not too hard to design (Evans *et al.*, 1991), ideally they should have some flexibility in order to accommodate chain motion and resultant strain.

By using a 1,2,3-trisubstituted phenyl ring and 1,2-ethane linkers it was hoped to get some flexibility as well as enforcing a re-entrant structure. In order to determine suitable polymer backbones, model oligomers were synthesized for structural analysis and monomer (I) was obtained from the hydrogenation of the Wittig-produced diene.

In (I), the biphenyl system is linked symmetrically at the 2 and 6-positions *via* two ethandiyl chains to two benzyloxyphenyl units. In the solid state, both the ethandiyl and benzyl ether linkages stayed *trans* - reinforcing the overall re-entrant structure of the central 1,2,3-phenyl linkage. The rings of the biphenyl group are almost orthogonal with a dihedral angle of 85.34 (8)° between them. The rings of the two benzyloxybenzene groups are inclined at 58.99 (10)° C1···C6/C9···C14 and 33.22 (13)° C31···C36/C39···C44 respectively.

In the crystal, molecules form inversion related dimers through C—H···O hydrogen bonds and are further linked into a three dimensional network by a series of C—H···π interactions. Fig 2, Table 1.

Experimental

2,6-Bis(4-benzyloxystyryl)biphenyl, 1, (0.56 g, 1.0 mmol) and 10% palladium on charcoal (0.10 g, 0.1 mmol) in ethyl acetate (50 *cm*3) were rocked under hydrogen at 40 psi at room temperature for 48 h. The solution was filtered through a short celite pad and concentrated *in vacuo* to yield a yellow solid. Flash chromatography, eluting in hexane-ethyl acetate (4:1), afforded 2,6-bis[2-(4-benzyloxyphenyl)ethyl]biphenyl (0.23 g, 41%) as a white solid: mp 133–134 °C [Found: C, 87.3%; H, 6.65%; *M*+ 574.2872 (ESI). C42H38O2 requires C, 87.8%; H, 6.7%; *M*+ 574.2862]; νmax(KBr)/cm$_{-1}$ 3029 2956 2921 2865 (C—H), 1611 1582 1513 (aromatic), 1455, 1246, 1175, 1025; δH(400 MHz; $CDCl_3$) 7.39 (10*H*, m, ArH), 7.35 (2*H*, m, ArH), 7.31 (2*H*, m, ArH), 7.16 (1*H*, s, ArH), 6.78 (8*H*, m, ArH), 5.00 (4*H*, s, CH2O), 2.59 (8*H*, m, CH2CH2); δC(101 MHz; $CDCl_3$) 156.9, 141.4, 140.1, 139.8, 137.2, 134.4, 129.6, 129.2, 128.5, 128.1, 127.8, 127.4, 126.8, 114.6, 70.0 (OCH_2), 37.0 (CH_2CH_2), 36.5 (CH_2CH_2). Colourless crystals of (I) were obtained as needles from ethyl acetate layered with hexane.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso}=1.2U_{eq} (C) for aromatic and 0.99 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 groups. In the final difference Fourier map, two peaks of approximately 0.7 e $Å^{-3}$ are found close to C7 and O8 but no chemical significance could be attached to them.

Figures

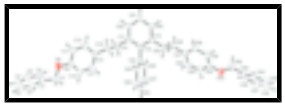


Fig. 1. The structure of (I) showing the atom numbering with ellipsoids drawn at the 50% probability level.

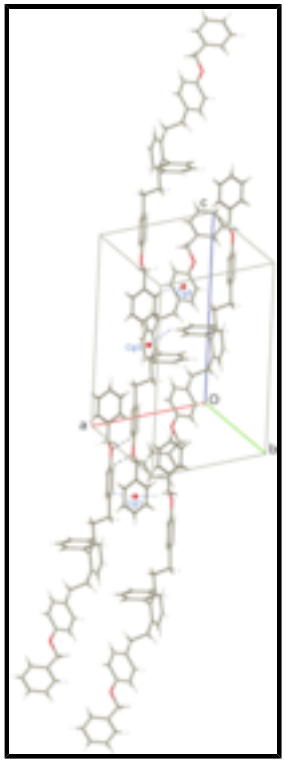


Fig. 2. Crystal packing for (I) with hydrogen bonds and C—H···π interactions drawn as dashed lines. Filled circles represent centroids of the benzene rings.

2,6-Bis[2-(4-benzyloxyphenyl)ethyl]biphenyl

Crystal data

$C_{42}H_{38}O_2$	Z = 2
M_r = 574.72	F_{000} = 612
Triclinic, $P\overline{1}$	D_x = 1.183 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.0431 (3) Å	Cell parameters from 12508 reflections
b = 10.2145 (3) Å	θ = 1.0–27.5º
c = 16.4136 (5) Å	μ = 0.07 mm^{-1}

α = 100.213 (2)º	T = 180 (2) K
β = 98.218 (2)º	Plate, colourless
γ = 98.642 (2)º	0.30 × 0.18 × 0.05 mm
V = 1613.22 (8) Å^3	

Data collection

Nonius KappaCCD diffractometer	7345 independent reflections
Radiation source: fine-focus sealed tube	5114 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 180(2) K	θ_{max} = 27.5º
Thin–slice ω and φ scans	θ_{min} = 3.6º
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	h = −13→12
T_{min} = 0.971, T_{max} = 0.980	k = −13→13
22105 measured reflections	l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.066	H-atom parameters constrained
$wR(F^2)$ = 0.169	$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.8567P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.005
7345 reflections	$\Delta\rho_{max}$ = 0.73 e Å^{-3}
397 parameters	$\Delta\rho_{min}$ = −0.44 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	1.0625 (3)	0.8508 (2)	−0.04760 (14)	0.0504 (6)

C2	0.9489 (2)	0.8225 (2)	−0.11049 (17)	0.0565 (6)
H2A	0.8618	0.7890	−0.0985	0.068*
C3	0.9602 (3)	0.8420 (2)	−0.19012 (16)	0.0593 (7)
H3A	0.8811	0.8228	−0.2326	0.071*
C4	1.0842 (3)	0.8888 (3)	−0.20805 (16)	0.0618 (7)
H4A	1.0918	0.9019	−0.2632	0.074*
C5	1.1969 (3)	0.9168 (3)	−0.1476 (2)	0.0681 (8)
H5A	1.2834	0.9494	−0.1606	0.082*
C6	1.1873 (3)	0.8983 (3)	−0.06724 (17)	0.0610 (7)
H6A	1.2671	0.9183	−0.0252	0.073*
C7	1.0563 (3)	0.8383 (3)	0.04239 (17)	0.0665 (7)
H7A	1.1471	0.8740	0.0781	0.080*
H7B	0.9896	0.8912	0.0645	0.080*
O8	1.0169 (2)	0.70361 (19)	0.04364 (12)	0.0808 (6)
C9	0.9942 (3)	0.6682 (3)	0.11879 (15)	0.0539 (6)
C10	1.0227 (2)	0.7547 (2)	0.19627 (16)	0.0537 (6)
H10A	1.0600	0.8475	0.2014	0.064*
C11	0.9958 (2)	0.7036 (2)	0.26760 (14)	0.0468 (5)
H11A	1.0156	0.7627	0.3212	0.056*
C12	0.94126 (19)	0.5692 (2)	0.26109 (12)	0.0374 (4)
C13	0.9127 (3)	0.4867 (2)	0.18170 (14)	0.0516 (6)
H13A	0.8740	0.3940	0.1757	0.062*
C14	0.9387 (3)	0.5350 (3)	0.11136 (16)	0.0634 (7)
H14A	0.9182	0.4760	0.0578	0.076*
C15	0.91479 (19)	0.5109 (2)	0.33682 (13)	0.0399 (5)
H15A	0.9742	0.5691	0.3876	0.048*
H15B	0.9404	0.4202	0.3304	0.048*
C16	0.76568 (18)	0.49849 (19)	0.34982 (11)	0.0323 (4)
H16A	0.7423	0.5899	0.3622	0.039*
H16B	0.7049	0.4472	0.2974	0.039*
C17	0.74155 (16)	0.42761 (18)	0.42112 (11)	0.0285 (4)
C18	0.74898 (16)	0.49903 (17)	0.50373 (11)	0.0270 (4)
C19	0.73258 (17)	0.42965 (18)	0.56915 (11)	0.0287 (4)
C20	0.70909 (18)	0.28851 (19)	0.55089 (12)	0.0337 (4)
H20A	0.6985	0.2405	0.5948	0.040*
C21	0.70094 (19)	0.21757 (19)	0.46983 (12)	0.0359 (4)
H21A	0.6846	0.1215	0.4583	0.043*
C22	0.71646 (18)	0.28627 (19)	0.40563 (12)	0.0335 (4)
H22A	0.7100	0.2368	0.3500	0.040*
C23	0.77486 (18)	0.65079 (17)	0.52238 (10)	0.0286 (4)
C24	0.90739 (19)	0.72428 (19)	0.53862 (12)	0.0355 (4)
H24A	0.9825	0.6779	0.5369	0.043*
C25	0.9312 (2)	0.8645 (2)	0.55727 (13)	0.0440 (5)
H25A	1.0223	0.9135	0.5687	0.053*
C26	0.8231 (2)	0.9328 (2)	0.55932 (13)	0.0481 (5)
H26A	0.8394	1.0289	0.5723	0.058*
C27	0.6912 (2)	0.8613 (2)	0.54248 (13)	0.0449 (5)
H27A	0.6166	0.9084	0.5435	0.054*
C28	0.6665 (2)	0.7211 (2)	0.52408 (12)	0.0368 (4)

H28A	0.5751	0.6728	0.5126	0.044*
C29	0.73770 (18)	0.50279 (19)	0.65846 (11)	0.0323 (4)
H29A	0.7910	0.5953	0.6668	0.039*
H29B	0.7857	0.4549	0.6977	0.039*
C30	0.5957 (2)	0.5116 (2)	0.67939 (12)	0.0417 (5)
H30A	0.5488	0.5614	0.6409	0.050*
H30B	0.5418	0.4190	0.6694	0.050*
C31	0.59842 (19)	0.5813 (2)	0.76926 (12)	0.0386 (4)
C32	0.5546 (2)	0.7035 (2)	0.78777 (13)	0.0449 (5)
H32A	0.5268	0.7472	0.7433	0.054*
C33	0.5504 (2)	0.7636 (2)	0.86958 (13)	0.0477 (5)
H33A	0.5187	0.8470	0.8807	0.057*
C34	0.5919 (2)	0.7027 (2)	0.93522 (13)	0.0423 (5)
C35	0.6418 (2)	0.5836 (2)	0.91888 (14)	0.0489 (5)
H35A	0.6744	0.5428	0.9637	0.059*
C36	0.6437 (2)	0.5239 (2)	0.83581 (14)	0.0461 (5)
H36A	0.6770	0.4414	0.8247	0.055*
O37	0.57941 (18)	0.76905 (16)	1.01376 (9)	0.0546 (4)
C38	0.6185 (2)	0.7105 (2)	1.08315 (13)	0.0486 (5)
H38A	0.7189	0.7159	1.0935	0.058*
H38B	0.5746	0.6140	1.0714	0.058*
C39	0.5748 (2)	0.7855 (2)	1.15913 (13)	0.0405 (5)
C40	0.4617 (3)	0.8461 (3)	1.15324 (16)	0.0568 (6)
H40A	0.4097	0.8432	1.0996	0.068*
C41	0.4231 (3)	0.9115 (3)	1.22520 (19)	0.0696 (8)
H41A	0.3447	0.9534	1.2210	0.084*
C42	0.4987 (3)	0.9157 (3)	1.30297 (18)	0.0741 (8)
H42A	0.4726	0.9604	1.3525	0.089*
C43	0.6112 (3)	0.8553 (3)	1.30865 (16)	0.0708 (8)
H43A	0.6635	0.8583	1.3622	0.085*
C44	0.6488 (3)	0.7907 (2)	1.23758 (14)	0.0535 (6)
H44A	0.7271	0.7488	1.2423	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0693 (15)	0.0448 (12)	0.0490 (13)	0.0197 (11)	0.0214 (11)	0.0242 (10)
C2	0.0458 (13)	0.0459 (13)	0.0817 (18)	0.0012 (10)	0.0177 (12)	0.0235 (12)
C3	0.0687 (16)	0.0458 (13)	0.0548 (15)	0.0080 (12)	−0.0095 (12)	0.0059 (11)
C4	0.092 (2)	0.0542 (15)	0.0516 (14)	0.0225 (14)	0.0245 (14)	0.0269 (12)
C5	0.0565 (15)	0.0621 (16)	0.098 (2)	0.0035 (12)	0.0314 (15)	0.0411 (15)
C6	0.0521 (14)	0.0575 (15)	0.0701 (17)	0.0041 (11)	−0.0069 (12)	0.0234 (13)
C7	0.0829 (19)	0.0562 (15)	0.0645 (16)	0.0079 (14)	0.0212 (14)	0.0207 (13)
O8	0.1388 (19)	0.0630 (12)	0.0708 (12)	0.0393 (12)	0.0610 (13)	0.0414 (10)
C9	0.0708 (16)	0.0608 (15)	0.0518 (14)	0.0327 (12)	0.0333 (12)	0.0330 (12)
C10	0.0473 (13)	0.0518 (13)	0.0716 (16)	0.0091 (10)	0.0173 (11)	0.0322 (12)
C11	0.0405 (11)	0.0545 (13)	0.0476 (12)	0.0068 (10)	0.0092 (9)	0.0163 (10)
C12	0.0322 (10)	0.0480 (11)	0.0418 (11)	0.0169 (8)	0.0138 (8)	0.0213 (9)

C13	0.0767 (16)	0.0423 (12)	0.0493 (13)	0.0229 (11)	0.0294 (12)	0.0198 (10)
C14	0.110 (2)	0.0508 (14)	0.0480 (13)	0.0344 (14)	0.0382 (14)	0.0226 (11)
C15	0.0328 (10)	0.0563 (13)	0.0385 (11)	0.0140 (9)	0.0107 (8)	0.0224 (9)
C16	0.0294 (9)	0.0399 (10)	0.0297 (9)	0.0095 (8)	0.0054 (7)	0.0098 (8)
C17	0.0217 (8)	0.0338 (9)	0.0318 (9)	0.0079 (7)	0.0051 (7)	0.0088 (7)
C18	0.0208 (8)	0.0294 (9)	0.0317 (9)	0.0052 (7)	0.0044 (7)	0.0084 (7)
C19	0.0220 (8)	0.0338 (9)	0.0317 (9)	0.0055 (7)	0.0049 (7)	0.0097 (7)
C20	0.0313 (9)	0.0340 (10)	0.0387 (10)	0.0050 (8)	0.0075 (8)	0.0147 (8)
C21	0.0345 (10)	0.0277 (9)	0.0451 (11)	0.0053 (8)	0.0042 (8)	0.0083 (8)
C22	0.0313 (9)	0.0349 (10)	0.0329 (9)	0.0074 (8)	0.0048 (7)	0.0024 (8)
C23	0.0316 (9)	0.0305 (9)	0.0249 (8)	0.0062 (7)	0.0046 (7)	0.0082 (7)
C24	0.0336 (10)	0.0355 (10)	0.0386 (10)	0.0047 (8)	0.0044 (8)	0.0138 (8)
C25	0.0468 (12)	0.0362 (11)	0.0445 (12)	−0.0030 (9)	−0.0012 (9)	0.0128 (9)
C26	0.0694 (15)	0.0280 (10)	0.0433 (12)	0.0065 (10)	0.0016 (11)	0.0066 (9)
C27	0.0549 (13)	0.0388 (11)	0.0450 (12)	0.0197 (10)	0.0102 (10)	0.0086 (9)
C28	0.0352 (10)	0.0382 (11)	0.0394 (10)	0.0111 (8)	0.0088 (8)	0.0085 (8)
C29	0.0296 (9)	0.0377 (10)	0.0304 (9)	0.0041 (8)	0.0055 (7)	0.0105 (8)
C30	0.0323 (10)	0.0532 (13)	0.0378 (11)	0.0060 (9)	0.0075 (8)	0.0044 (9)
C31	0.0298 (10)	0.0466 (11)	0.0383 (11)	0.0021 (8)	0.0090 (8)	0.0074 (9)
C32	0.0419 (11)	0.0568 (13)	0.0374 (11)	0.0141 (10)	0.0052 (9)	0.0100 (10)
C33	0.0524 (13)	0.0510 (13)	0.0414 (12)	0.0172 (10)	0.0088 (10)	0.0064 (10)
C34	0.0450 (12)	0.0455 (12)	0.0365 (11)	0.0059 (9)	0.0148 (9)	0.0040 (9)
C35	0.0620 (14)	0.0513 (13)	0.0409 (12)	0.0156 (11)	0.0190 (10)	0.0167 (10)
C36	0.0543 (13)	0.0420 (12)	0.0476 (12)	0.0129 (10)	0.0211 (10)	0.0108 (10)
O37	0.0773 (11)	0.0561 (10)	0.0343 (8)	0.0223 (8)	0.0144 (7)	0.0073 (7)
C38	0.0509 (13)	0.0589 (14)	0.0421 (12)	0.0187 (11)	0.0142 (10)	0.0139 (10)
C39	0.0440 (11)	0.0396 (11)	0.0388 (11)	0.0039 (9)	0.0134 (9)	0.0088 (9)
C40	0.0518 (14)	0.0674 (16)	0.0504 (14)	0.0153 (12)	0.0079 (11)	0.0069 (12)
C41	0.0597 (16)	0.0670 (17)	0.084 (2)	0.0177 (13)	0.0278 (15)	0.0017 (15)
C42	0.095 (2)	0.0669 (18)	0.0559 (16)	0.0004 (16)	0.0405 (16)	−0.0080 (13)
C43	0.097 (2)	0.0713 (18)	0.0383 (13)	0.0064 (16)	0.0100 (14)	0.0059 (12)
C44	0.0592 (14)	0.0558 (14)	0.0474 (13)	0.0101 (11)	0.0089 (11)	0.0163 (11)

Geometric parameters (Å, °)

C1—C6	1.377 (3)	C23—C24	1.390 (3)
C1—C2	1.382 (3)	C23—C28	1.392 (2)
C1—C7	1.514 (3)	C24—C25	1.387 (3)
C2—C3	1.375 (4)	C24—H24A	0.9500
C2—H2A	0.9500	C25—C26	1.378 (3)
C3—C4	1.357 (4)	C25—H25A	0.9500
C3—H3A	0.9500	C26—C27	1.377 (3)
C4—C5	1.352 (4)	C26—H26A	0.9500
C4—H4A	0.9500	C27—C28	1.386 (3)
C5—C6	1.380 (4)	C27—H27A	0.9500
C5—H5A	0.9500	C28—H28A	0.9500
C6—H6A	0.9500	C29—C30	1.525 (3)
C7—O8	1.378 (3)	C29—H29A	0.9900
C7—H7A	0.9900	C29—H29B	0.9900

C7—H7B	0.9900	C30—C31	1.515 (3)
O8—C9	1.385 (3)	C30—H30A	0.9900
C9—C14	1.368 (4)	C30—H30B	0.9900
C9—C10	1.379 (3)	C31—C36	1.382 (3)
C10—C11	1.407 (3)	C31—C32	1.384 (3)
C10—H10A	0.9500	C32—C33	1.383 (3)
C11—C12	1.379 (3)	C32—H32A	0.9500
C11—H11A	0.9500	C33—C34	1.381 (3)
C12—C13	1.386 (3)	C33—H33A	0.9500
C12—C15	1.510 (3)	C34—O37	1.378 (2)
C13—C14	1.376 (3)	C34—C35	1.381 (3)
C13—H13A	0.9500	C35—C36	1.396 (3)
C14—H14A	0.9500	C35—H35A	0.9500
C15—C16	1.532 (3)	C36—H36A	0.9500
C15—H15A	0.9900	O37—C38	1.412 (3)
C15—H15B	0.9900	C38—C39	1.501 (3)
C16—C17	1.510 (2)	C38—H38A	0.9900
C16—H16A	0.9900	C38—H38B	0.9900
C16—H16B	0.9900	C39—C40	1.373 (3)
C17—C22	1.398 (2)	C39—C44	1.380 (3)
C17—C18	1.407 (2)	C40—C41	1.386 (4)
C18—C19	1.403 (2)	C40—H40A	0.9500
C18—C23	1.501 (2)	C41—C42	1.379 (4)
C19—C20	1.396 (2)	C41—H41A	0.9500
C19—C29	1.513 (2)	C42—C43	1.366 (4)
C20—C21	1.382 (3)	C42—H42A	0.9500
C20—H20A	0.9500	C43—C44	1.367 (4)
C21—C22	1.380 (3)	C43—H43A	0.9500
C21—H21A	0.9500	C44—H44A	0.9500
C22—H22A	0.9500		
C6—C1—C2	118.1 (2)	C24—C23—C28	118.52 (17)
C6—C1—C7	118.3 (2)	C24—C23—C18	120.83 (16)
C2—C1—C7	123.6 (2)	C28—C23—C18	120.64 (16)
C3—C2—C1	120.8 (2)	C25—C24—C23	120.76 (18)
C3—C2—H2A	119.6	C25—C24—H24A	119.6
C1—C2—H2A	119.6	C23—C24—H24A	119.6
C4—C3—C2	120.1 (2)	C26—C25—C24	120.11 (19)
C4—C3—H3A	120.0	C26—C25—H25A	119.9
C2—C3—H3A	120.0	C24—C25—H25A	119.9
C5—C4—C3	120.1 (2)	C27—C26—C25	119.73 (19)
C5—C4—H4A	119.9	C27—C26—H26A	120.1
C3—C4—H4A	119.9	C25—C26—H26A	120.1
C4—C5—C6	120.5 (2)	C26—C27—C28	120.54 (19)
C4—C5—H5A	119.7	C26—C27—H27A	119.7
C6—C5—H5A	119.7	C28—C27—H27A	119.7
C1—C6—C5	120.3 (2)	C27—C28—C23	120.33 (19)
C1—C6—H6A	119.8	C27—C28—H28A	119.8
C5—C6—H6A	119.8	C23—C28—H28A	119.8
O8—C7—C1	108.3 (2)	C19—C29—C30	112.53 (15)

O8—C7—H7A	110.0	C19—C29—H29A	109.1
C1—C7—H7A	110.0	C30—C29—H29A	109.1
O8—C7—H7B	110.0	C19—C29—H29B	109.1
C1—C7—H7B	110.0	C30—C29—H29B	109.1
H7A—C7—H7B	108.4	H29A—C29—H29B	107.8
C7—O8—C9	118.7 (2)	C31—C30—C29	113.37 (16)
C14—C9—C10	120.3 (2)	C31—C30—H30A	108.9
C14—C9—O8	114.2 (2)	C29—C30—H30A	108.9
C10—C9—O8	125.5 (2)	C31—C30—H30B	108.9
C9—C10—C11	119.1 (2)	C29—C30—H30B	108.9
C9—C10—H10A	120.4	H30A—C30—H30B	107.7
C11—C10—H10A	120.4	C36—C31—C32	117.61 (19)
C12—C11—C10	121.1 (2)	C36—C31—C30	120.93 (19)
C12—C11—H11A	119.4	C32—C31—C30	121.46 (19)
C10—C11—H11A	119.4	C33—C32—C31	121.4 (2)
C11—C12—C13	117.58 (19)	C33—C32—H32A	119.3
C11—C12—C15	122.25 (19)	C31—C32—H32A	119.3
C13—C12—C15	120.16 (19)	C34—C33—C32	120.2 (2)
C14—C13—C12	122.0 (2)	C34—C33—H33A	119.9
C14—C13—H13A	119.0	C32—C33—H33A	119.9
C12—C13—H13A	119.0	O37—C34—C35	125.08 (19)
C9—C14—C13	119.8 (2)	O37—C34—C33	115.36 (19)
C9—C14—H14A	120.1	C35—C34—C33	119.56 (19)
C13—C14—H14A	120.1	C34—C35—C36	119.3 (2)
C12—C15—C16	113.56 (15)	C34—C35—H35A	120.4
C12—C15—H15A	108.9	C36—C35—H35A	120.4
C16—C15—H15A	108.9	C31—C36—C35	121.8 (2)
C12—C15—H15B	108.9	C31—C36—H36A	119.1
C16—C15—H15B	108.9	C35—C36—H36A	119.1
H15A—C15—H15B	107.7	C34—O37—C38	117.91 (17)
C17—C16—C15	111.51 (14)	O37—C38—C39	108.87 (17)
C17—C16—H16A	109.3	O37—C38—H38A	109.9
C15—C16—H16A	109.3	C39—C38—H38A	109.9
C17—C16—H16B	109.3	O37—C38—H38B	109.9
C15—C16—H16B	109.3	C39—C38—H38B	109.9
H16A—C16—H16B	108.0	H38A—C38—H38B	108.3
C22—C17—C18	118.59 (16)	C40—C39—C44	119.0 (2)
C22—C17—C16	119.16 (16)	C40—C39—C38	122.1 (2)
C18—C17—C16	122.20 (16)	C44—C39—C38	118.9 (2)
C19—C18—C17	120.59 (16)	C39—C40—C41	120.2 (2)
C19—C18—C23	119.48 (15)	C39—C40—H40A	119.9
C17—C18—C23	119.92 (15)	C41—C40—H40A	119.9
C20—C19—C18	118.82 (16)	C42—C41—C40	119.8 (3)
C20—C19—C29	119.04 (16)	C42—C41—H41A	120.1
C18—C19—C29	122.13 (16)	C40—C41—H41A	120.1
C21—C20—C19	120.95 (17)	C43—C42—C41	119.8 (2)
C21—C20—H20A	119.5	C43—C42—H42A	120.1
C19—C20—H20A	119.5	C41—C42—H42A	120.1
C22—C21—C20	120.01 (17)	C42—C43—C44	120.2 (3)

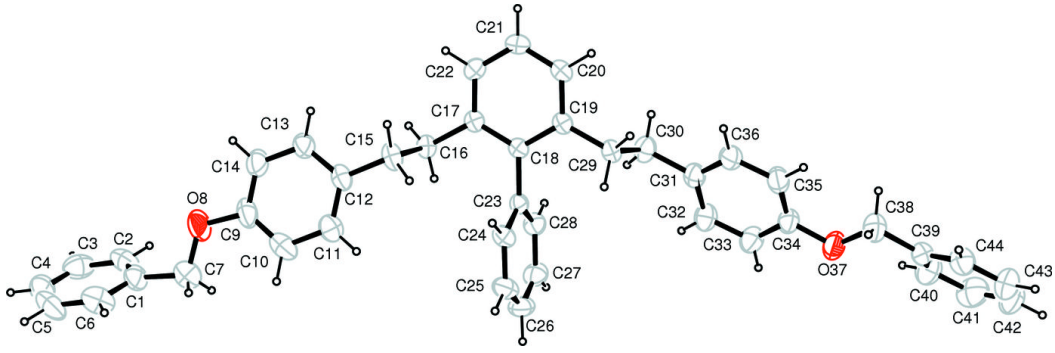
C22—C21—H21A	120.0	C42—C43—H43A	119.9
C20—C21—H21A	120.0	C44—C43—H43A	119.9
C21—C22—C17	121.04 (17)	C43—C44—C39	120.9 (2)
C21—C22—H22A	119.5	C43—C44—H44A	119.5
C17—C22—H22A	119.5	C39—C44—H44A	119.5
C6—C1—C2—C3	−0.4 (4)	C16—C17—C22—C21	176.61 (16)
C7—C1—C2—C3	176.8 (2)	C19—C18—C23—C24	94.7 (2)
C1—C2—C3—C4	0.5 (4)	C17—C18—C23—C24	−85.2 (2)
C2—C3—C4—C5	−0.2 (4)	C19—C18—C23—C28	−85.1 (2)
C3—C4—C5—C6	0.0 (4)	C17—C18—C23—C28	95.0 (2)
C2—C1—C6—C5	0.2 (4)	C28—C23—C24—C25	0.9 (3)
C7—C1—C6—C5	−177.2 (2)	C18—C23—C24—C25	−178.87 (17)
C4—C5—C6—C1	0.1 (4)	C23—C24—C25—C26	−0.5 (3)
C6—C1—C7—O8	−116.2 (3)	C24—C25—C26—C27	−0.2 (3)
C2—C1—C7—O8	66.5 (3)	C25—C26—C27—C28	0.5 (3)
C1—C7—O8—C9	−175.3 (2)	C26—C27—C28—C23	0.0 (3)
C7—O8—C9—C14	171.9 (2)	C24—C23—C28—C27	−0.7 (3)
C7—O8—C9—C10	−8.0 (4)	C18—C23—C28—C27	179.12 (17)
C14—C9—C10—C11	1.0 (4)	C20—C19—C29—C30	−82.1 (2)
O8—C9—C10—C11	−179.1 (2)	C18—C19—C29—C30	97.1 (2)
C9—C10—C11—C12	−0.3 (3)	C19—C29—C30—C31	178.50 (17)
C10—C11—C12—C13	−0.6 (3)	C29—C30—C31—C36	−66.3 (3)
C10—C11—C12—C15	178.38 (19)	C29—C30—C31—C32	114.4 (2)
C11—C12—C13—C14	0.8 (3)	C36—C31—C32—C33	−2.8 (3)
C15—C12—C13—C14	−178.2 (2)	C30—C31—C32—C33	176.6 (2)
C10—C9—C14—C13	−0.8 (4)	C31—C32—C33—C34	0.8 (3)
O8—C9—C14—C13	179.3 (2)	C32—C33—C34—O37	−178.05 (19)
C12—C13—C14—C9	−0.1 (4)	C32—C33—C34—C35	2.0 (3)
C11—C12—C15—C16	98.6 (2)	O37—C34—C35—C36	177.3 (2)
C13—C12—C15—C16	−82.4 (2)	C33—C34—C35—C36	−2.7 (3)
C12—C15—C16—C17	174.56 (17)	C32—C31—C36—C35	2.0 (3)
C15—C16—C17—C22	−83.3 (2)	C30—C31—C36—C35	−177.3 (2)
C15—C16—C17—C18	94.1 (2)	C34—C35—C36—C31	0.7 (3)
C22—C17—C18—C19	0.5 (2)	C35—C34—O37—C38	−0.9 (3)
C16—C17—C18—C19	−176.86 (15)	C33—C34—O37—C38	179.1 (2)
C22—C17—C18—C23	−179.60 (15)	C34—O37—C38—C39	−170.58 (18)
C16—C17—C18—C23	3.1 (2)	O37—C38—C39—C40	30.2 (3)
C17—C18—C19—C20	0.2 (2)	O37—C38—C39—C44	−151.5 (2)
C23—C18—C19—C20	−179.76 (15)	C44—C39—C40—C41	0.1 (4)
C17—C18—C19—C29	−179.03 (15)	C38—C39—C40—C41	178.4 (2)
C23—C18—C19—C29	1.1 (2)	C39—C40—C41—C42	0.0 (4)
C18—C19—C20—C21	−0.5 (3)	C40—C41—C42—C43	0.0 (4)
C29—C19—C20—C21	178.72 (16)	C41—C42—C43—C44	−0.1 (4)
C19—C20—C21—C22	0.2 (3)	C42—C43—C44—C39	0.2 (4)
C20—C21—C22—C17	0.5 (3)	C40—C39—C44—C43	−0.2 (4)
C18—C17—C22—C21	−0.8 (3)	C38—C39—C44—C43	−178.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14A···O8^{i}	0.95	2.48	3.326 (4)	149
C2—H2A···Cg5^{ii}	0.95	2.78	3.644 (2)	152
C7—H7B···Cg1^{iii}	0.99	2.68	3.575 (3)	150
C13—H13A···Cg1^{iv}	0.95	2.82	3.620 (2)	143
C28—H28A···Cg3^{v}	0.95	2.98	3.865 (2)	155

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

Fig. 1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C43
C1
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C40
C5
C6
C26
C41
C42

Fig. 2