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1,4-Bis[(3,5-dimethoxyphenyl)ethynyl]-benzene

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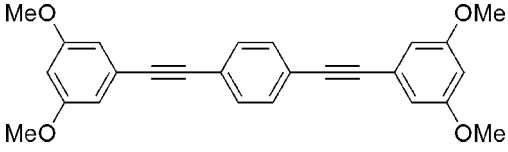
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.140; data-to-parameter ratio = 17.1.

The title compound, $C_{26}H_{22}O_4$, is a derivative of 1,4-bis(phenylethynyl)benzene substituted by four methoxy groups on the terminal benzene rings. The molecule is almost planar with an r.m.s. deviation of 0.266 Å. The dihedral angles between the two terminal benzene rings and the central benzene ring are 7.96 (6) and 13.32 (7)°. In the crystal structure, molecules aggregate *via* C—H···O interactions, forming molecular tapes along the *a* axis, which aggregate to form a herring-bone structure.

Related literature

For the crystal structure of 1,4-bis[(2,6-dimethoxyphenyl)-ethynyl]benzene, see: Ono *et al.* (2008). For related sructures, including a 1,4-bis(phenylethynyl)benzene system, see: Watt *et al.* (2004); Li *et al.* (1998); Filatov & Petrukhina (2005).



Experimental

Crystal data

$C_{26}H_{22}O_4$
M_r = 398.44
Monoclinic, $P2_1/a$
a = 8.8980 (5) Å
b = 19.4610 (8) Å
c = 12.2820 (5) Å
β = 100.607 (1)°
V = 2090.46 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (1) K
0.30 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: none
15238 measured reflections
4638 independent reflections
3914 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.11
4638 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O4^{i}	0.95	2.42	3.3511 (17)	167
C14—H14···O2^{ii}	0.95	2.37	3.2758 (16)	160

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

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2753).

References

Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Filatov, A. S. & Petrukhina, M. A. (2005). *Acta Cryst.* C**61**, o193–o194.
Li, H., Powell, D. R., Firman, T. K. & West, R. (1998). *Macromolecules*, **31**, 1093–1098.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Ono, K., Tsukamoto, K., Tomura, M. & Saito, K. (2008). *Acta Cryst.* E**64**, o1069.
Rigaku (2001). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Watt, S. W., Dai, C., Scott, A. J., Burke, J. M., Thomas, R. Ll., Collings, J. C., Viney, C., Clegg, W. & Marder, T. B. (2004). *Angew. Chem. Int. Ed.* **43**, 3061–3063.

supplementary materials

Acta Cryst. (2009). E**65**, o346 [**doi:10.1107/S160053680900155X**]

1,4-Bis[(3,5-dimethoxyphenyl)ethynyl]benzene

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Comment

The synthetic research of ethynylated aromatic compounds has attracted considerable attention because of interests in their molecular structures, optical properties, and molecular electronics. Among these ethynylated aromatic compounds, 1,4-bis(phenylethynyl)benzene derivatives have been extensively studied. These compounds have stiff, linear molecular structures and are used as building blocks in the applications. Recently, we found that 1,4-bis[(2,6-dimethoxyphenyl)ethynyl]benzene, (II), formed a zigzag molecular network in the crystal (Ono *et al.*, 2008). The crystal structure is different from those of 1,4-bis(phenylethynyl)benzene derivatives (Watt *et al.*, 2004; Li *et al.*, 1998; Filatov & Petrukhina, 2005). With regard to this, we investigated the molecular and crystal structure of the title compound, (I), which is a regioisomer of (II). The substitution effect of four methoxy groups at the terminal benzene rings was studied.

The molecular structure of (I) is shown in Fig. 1. The molecule is almost planar with an r.m.s deviation of 0.266 Å. The dihedral angles between the terminal benzene rings and the central benzene ring are 7.96 (6)° (C1–C6) and 13.32 (7)° (C17–C22). The methoxy groups are coplanar with the attached benzene rings.

The crystal structure is characterized by a molecular tape along the *a* axis formed by C—H···O interactions (Table 1 and Fig. 2). The molecular tapes aggregate to form a herring-bone-type structure, as shown in Fig.3. The crystal structure of (I) is different from that of (II). The crystal structures of (I) and (II) indicate that the methoxy groups at terminal benzene rings play an important role in the crystal packing.

Experimental

The title compound (I) was prepared as follows: Tetrakis(triphenylphosphine)palladium(0) [$Pd(PPh_3)_4$] (52 mg, 0.045 mmol) was added to a mixture of 1-ethynyl-3,5-dimethoxybenzene (0.39 g, 2.4 mmol), 1,4-diiodobenzene (0.39 g, 1.2 mmol) and copper(I) iodide (5 mg, 0.03 mmol) in dry triethylamine (7 ml) under nitrogen. The reaction mixture was stirred for 18 h at 353 K. After removal of the solvent, dichloromethane (20 ml) and aqueous disodium ethylenediaminetetraacetate (Na_2edta) solution (5%, 20 ml) were added. The organic layer was separated and washed with water (20 ml). The organic solution was dried over Na_2SO_4 and concentrated. The residue was chromatographed on silica gel (CH_2Cl_2) to afford the title compound (0.23 g, 49%) as a yellow powder. Yellow crystals of the compound, suitable for X-ray analysis were grown from an ethanol solution.

Refinement

All H atoms were placed in geometrically calculated positions, with C-H = 0.95 (aromatic) and 0.98 Å (methyl) and U_{iso}(H) = 1.2U_{eq}(C) (aromatic) and 1.5U_{eq}(C) (methyl), and refined using a riding model.

Figures

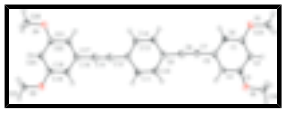

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms and H atoms are shown as small spheres of arbitrary radii.

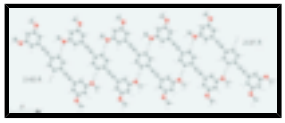

Fig. 2. Partial packing diagram of (I), showing a molecular tape along the *a* axis.

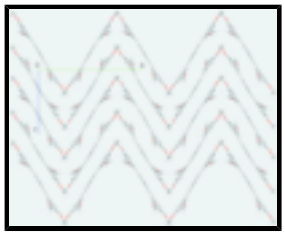

Fig. 3. The packing diagram of (I), showing herringbone-type network on the *bc* plane.

1,4-Bis[(3,5-dimethoxyphenyl)ethynyl]benzene

Crystal data

$C_{26}H_{22}O_4$	F_{000} = 840
M_r = 398.44	D_x = 1.266 Mg m^{-3}
Monoclinic, $P2_1/a$	Melting point: 431 K
Hall symbol: -P 2yab	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.8980 (5) Å	Cell parameters from 5437 reflections
b = 19.4610 (8) Å	θ = 3.1–27.5º
c = 12.2820 (5) Å	μ = 0.09 mm^{-1}
β = 100.607 (1)º	T = 173 (1) K
V = 2090.46 (17) Å^3	Block, yellow
Z = 4	0.30 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer	3914 reflections with $I > 2\sigma(I)$
Monochromator: Graphite Monochromator	R_{int} = 0.024
Detector resolution: 14.7059 pixels mm^{-1}	θ_{max} = 27.5º
T = 173(1) K	θ_{min} = 3.1º
φ and ω scans	h = −11→10
Absorption correction: none	k = −22→25
15238 measured reflections	l = −15→12
4638 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.140$

$S = 1.11$

4638 reflections

271 parameters

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.1522P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.26$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: none

Special details

Experimental. IR (KBr, cm^{-1}): 1605, 1580, 1345, 1254, 1202, 1161, 1065, 841; ^{1}H NMR ($CDCl_3$, δ p.p.m.): 3.81 (s, 12H), 6.48 (t, J = 2.3 Hz, 2H), 6.70 (d, J = 2.3 Hz, 4H), 7.51 (s, 4H); ^{13}C NMR ($CDCl_3$, δ p.p.m.): 55.3, 88.6, 91.3, 102.0, 109.4, 123.0, 124.3, 131.6, 160.6; MS (EI): m/*z* 398 (M^+), 199.

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 $F^2 > \sigma(F^2)$ 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	0.04347 (14)	0.17522 (6)	0.71287 (10)	0.0266 (3)
C2	−0.11459 (14)	0.17481 (6)	0.67760 (11)	0.0266 (3)
H2	−0.1799	0.1980	0.7185	0.032*
C3	−0.17430 (13)	0.13932 (6)	0.58033 (11)	0.0265 (3)
C4	−0.07979 (14)	0.10623 (6)	0.51948 (11)	0.0277 (3)
H4	−0.1225	0.0824	0.4535	0.033*
C5	0.07839 (14)	0.10787 (6)	0.55512 (10)	0.0261 (3)
C6	0.14059 (14)	0.14194 (6)	0.65309 (11)	0.0283 (3)
H6	0.2480	0.1424	0.6787	0.034*
C7	0.17340 (14)	0.07642 (6)	0.48619 (11)	0.0288 (3)
C8	0.24292 (14)	0.05168 (7)	0.42138 (11)	0.0288 (3)
C9	0.32492 (14)	0.02180 (6)	0.34289 (10)	0.0262 (3)
C10	0.24597 (14)	−0.01164 (7)	0.24864 (11)	0.0286 (3)
H10	0.1377	−0.0150	0.2371	0.034*
C11	0.32439 (14)	−0.03986 (7)	0.17214 (11)	0.0303 (3)
H11	0.2695	−0.0621	0.1081	0.036*
C12	0.48372 (14)	−0.03594 (6)	0.18839 (10)	0.0273 (3)
C13	0.56275 (14)	−0.00329 (6)	0.28348 (11)	0.0297 (3)
H13	0.6712	−0.0009	0.2959	0.036*

C14	0.48439 (14)	0.02550 (7)	0.35943 (11)	0.0295 (3)
H14	0.5392	0.0479	0.4233	0.035*
C15	0.56748 (14)	−0.06453 (7)	0.10994 (11)	0.0305 (3)
C16	0.64138 (15)	−0.08764 (7)	0.04662 (11)	0.0313 (3)
C17	0.73414 (14)	−0.11338 (6)	−0.02860 (11)	0.0289 (3)
C18	0.67256 (14)	−0.15780 (7)	−0.11433 (11)	0.0309 (3)
H18	0.5689	−0.1720	−0.1231	0.037*
C19	0.76419 (14)	−0.18118 (7)	−0.18695 (11)	0.0289 (3)
C20	0.91672 (14)	−0.16179 (7)	−0.17484 (11)	0.0289 (3)
H20	0.9792	−0.1787	−0.2238	0.035*
C21	0.97568 (14)	−0.11696 (7)	−0.08931 (11)	0.0310 (3)
C22	0.88622 (14)	−0.09254 (7)	−0.01627 (11)	0.0316 (3)
H22	0.9283	−0.0619	0.0416	0.038*
C23	0.02302 (18)	0.24526 (8)	0.87014 (12)	0.0434 (4)
H23A	0.0889	0.2677	0.9328	0.065*
H23B	−0.0440	0.2122	0.8980	0.065*
H23C	−0.0392	0.2800	0.8247	0.065*
C24	−0.43253 (15)	0.17035 (8)	0.58918 (13)	0.0409 (4)
H24A	−0.5365	0.1618	0.5488	0.061*
H24B	−0.4108	0.2197	0.5890	0.061*
H24C	−0.4236	0.1543	0.6657	0.061*
C25	0.77935 (17)	−0.24753 (8)	−0.34851 (12)	0.0398 (3)
H25A	0.7151	−0.2772	−0.4025	0.060*
H25B	0.8679	−0.2737	−0.3107	0.060*
H25C	0.8146	−0.2082	−0.3868	0.060*
C26	1.22202 (17)	−0.11600 (9)	−0.14105 (15)	0.0506 (4)
H26A	1.3229	−0.0950	−0.1178	0.076*
H26B	1.1803	−0.1025	−0.2175	0.076*
H26C	1.2316	−0.1661	−0.1366	0.076*
O1	0.11541 (10)	0.21008 (5)	0.80454 (8)	0.0360 (2)
O2	−0.32622 (10)	0.13442 (5)	0.53688 (8)	0.0352 (2)
O3	0.69301 (10)	−0.22363 (5)	−0.26936 (9)	0.0396 (3)
O4	1.12292 (11)	−0.09341 (6)	−0.07075 (9)	0.0477 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0340 (6)	0.0247 (6)	0.0213 (6)	0.0006 (5)	0.0059 (5)	−0.0006 (5)
C2	0.0318 (6)	0.0241 (6)	0.0263 (7)	0.0011 (5)	0.0113 (5)	−0.0004 (5)
C3	0.0273 (6)	0.0244 (6)	0.0287 (7)	−0.0013 (4)	0.0073 (5)	0.0015 (5)
C4	0.0345 (6)	0.0257 (6)	0.0235 (6)	−0.0007 (5)	0.0068 (5)	−0.0036 (5)
C5	0.0322 (6)	0.0232 (6)	0.0249 (6)	0.0034 (5)	0.0106 (5)	0.0016 (5)
C6	0.0280 (6)	0.0281 (6)	0.0291 (7)	0.0025 (5)	0.0058 (5)	−0.0005 (5)
C7	0.0314 (6)	0.0279 (6)	0.0277 (7)	0.0016 (5)	0.0071 (5)	−0.0007 (5)
C8	0.0324 (6)	0.0280 (6)	0.0266 (7)	0.0020 (5)	0.0069 (5)	−0.0004 (5)
C9	0.0309 (6)	0.0248 (6)	0.0243 (6)	0.0033 (5)	0.0089 (5)	0.0012 (5)
C10	0.0266 (6)	0.0331 (7)	0.0265 (7)	0.0027 (5)	0.0061 (5)	−0.0005 (5)
C11	0.0340 (6)	0.0338 (7)	0.0226 (6)	0.0014 (5)	0.0042 (5)	−0.0045 (5)

C12	0.0330 (6)	0.0269 (6)	0.0238 (6)	0.0043 (5)	0.0103 (5)	0.0000 (5)
C13	0.0277 (6)	0.0333 (7)	0.0293 (7)	0.0007 (5)	0.0083 (5)	−0.0012 (5)
C14	0.0325 (6)	0.0316 (6)	0.0248 (7)	−0.0015 (5)	0.0064 (5)	−0.0051 (5)
C15	0.0346 (6)	0.0303 (7)	0.0278 (7)	0.0033 (5)	0.0086 (5)	−0.0006 (5)
C16	0.0358 (6)	0.0316 (7)	0.0278 (7)	0.0036 (5)	0.0092 (5)	−0.0007 (5)
C17	0.0344 (6)	0.0299 (6)	0.0238 (6)	0.0062 (5)	0.0089 (5)	0.0002 (5)
C18	0.0286 (6)	0.0338 (7)	0.0322 (7)	−0.0007 (5)	0.0109 (5)	−0.0034 (6)
C19	0.0317 (6)	0.0294 (6)	0.0259 (7)	−0.0011 (5)	0.0065 (5)	−0.0044 (5)
C20	0.0296 (6)	0.0330 (7)	0.0255 (7)	0.0018 (5)	0.0091 (5)	−0.0038 (5)
C21	0.0286 (6)	0.0363 (7)	0.0285 (7)	−0.0008 (5)	0.0057 (5)	−0.0029 (5)
C22	0.0356 (7)	0.0348 (7)	0.0244 (7)	0.0003 (5)	0.0057 (5)	−0.0071 (5)
C23	0.0512 (8)	0.0486 (9)	0.0291 (8)	0.0112 (7)	0.0037 (6)	−0.0135 (7)
C24	0.0286 (6)	0.0471 (9)	0.0487 (9)	0.0001 (6)	0.0112 (6)	−0.0110 (7)
C25	0.0459 (8)	0.0429 (8)	0.0324 (8)	−0.0052 (6)	0.0121 (6)	−0.0150 (6)
C26	0.0339 (7)	0.0718 (12)	0.0499 (10)	−0.0131 (7)	0.0179 (7)	−0.0190 (8)
O1	0.0364 (5)	0.0429 (6)	0.0274 (5)	0.0056 (4)	0.0023 (4)	−0.0123 (4)
O2	0.0271 (4)	0.0380 (5)	0.0403 (6)	−0.0022 (4)	0.0062 (4)	−0.0102 (4)
O3	0.0361 (5)	0.0459 (6)	0.0390 (6)	−0.0091 (4)	0.0123 (4)	−0.0198 (5)
O4	0.0302 (5)	0.0698 (7)	0.0446 (7)	−0.0122 (5)	0.0112 (4)	−0.0260 (6)

Geometric parameters (Å, °)

C1—O1	1.3684 (15)	C17—C22	1.3940 (18)
C1—C6	1.3924 (16)	C17—C18	1.3942 (18)
C1—C2	1.3933 (17)	C18—C19	1.3911 (16)
C2—C3	1.3975 (18)	C18—H18	0.95
C2—H2	0.95	C19—O3	1.3683 (15)
C3—O2	1.3622 (15)	C19—C20	1.3900 (17)
C3—C4	1.3826 (16)	C20—C21	1.3917 (18)
C4—C5	1.3953 (17)	C20—H20	0.95
C4—H4	0.95	C21—O4	1.3670 (15)
C5—C6	1.3960 (18)	C21—C22	1.3882 (17)
C5—C7	1.4386 (16)	C22—H22	0.95
C6—H6	0.95	C23—O1	1.4274 (16)
C7—C8	1.1956 (17)	C23—H23A	0.98
C8—C9	1.4348 (16)	C23—H23B	0.98
C9—C14	1.3977 (17)	C23—H23C	0.98
C9—C10	1.3991 (18)	C24—O2	1.4213 (15)
C10—C11	1.3831 (17)	C24—H24A	0.98
C10—H10	0.95	C24—H24B	0.98
C11—C12	1.3969 (17)	C24—H24C	0.98
C11—H11	0.95	C25—O3	1.4236 (16)
C12—C13	1.3999 (18)	C25—H25A	0.98
C12—C15	1.4345 (16)	C25—H25B	0.98
C13—C14	1.3820 (17)	C25—H25C	0.98
C13—H13	0.95	C26—O4	1.4130 (17)
C14—H14	0.95	C26—H26A	0.98
C15—C16	1.1949 (18)	C26—H26B	0.98
C16—C17	1.4375 (17)	C26—H26C	0.98

O1—C1—C6	115.01 (10)	C19—C18—C17	119.46 (11)
O1—C1—C2	123.44 (11)	C19—C18—H18	120.3
C6—C1—C2	121.49 (11)	C17—C18—H18	120.3
C1—C2—C3	118.14 (11)	O3—C19—C20	123.57 (11)
C1—C2—H2	120.9	O3—C19—C18	115.19 (11)
C3—C2—H2	120.9	C20—C19—C18	121.24 (12)
O2—C3—C4	114.46 (11)	C19—C20—C21	118.42 (11)
O2—C3—C2	124.28 (11)	C19—C20—H20	120.8
C4—C3—C2	121.26 (11)	C21—C20—H20	120.8
C3—C4—C5	119.91 (11)	O4—C21—C22	115.05 (12)
C3—C4—H4	120.0	O4—C21—C20	123.55 (11)
C5—C4—H4	120.0	C22—C21—C20	121.40 (11)
C4—C5—C6	119.88 (11)	C21—C22—C17	119.40 (12)
C4—C5—C7	118.29 (11)	C21—C22—H22	120.3
C6—C5—C7	121.78 (11)	C17—C22—H22	120.3
C1—C6—C5	119.30 (11)	O1—C23—H23A	109.5
C1—C6—H6	120.4	O1—C23—H23B	109.5
C5—C6—H6	120.4	H23A—C23—H23B	109.5
C8—C7—C5	174.44 (14)	O1—C23—H23C	109.5
C7—C8—C9	179.42 (15)	H23A—C23—H23C	109.5
C14—C9—C10	119.07 (11)	H23B—C23—H23C	109.5
C14—C9—C8	120.64 (11)	O2—C24—H24A	109.5
C10—C9—C8	120.29 (11)	O2—C24—H24B	109.5
C11—C10—C9	120.50 (11)	H24A—C24—H24B	109.5
C11—C10—H10	119.8	O2—C24—H24C	109.5
C9—C10—H10	119.8	H24A—C24—H24C	109.5
C10—C11—C12	120.45 (11)	H24B—C24—H24C	109.5
C10—C11—H11	119.8	O3—C25—H25A	109.5
C12—C11—H11	119.8	O3—C25—H25B	109.5
C11—C12—C13	119.00 (11)	H25A—C25—H25B	109.5
C11—C12—C15	121.46 (11)	O3—C25—H25C	109.5
C13—C12—C15	119.54 (11)	H25A—C25—H25C	109.5
C14—C13—C12	120.58 (11)	H25B—C25—H25C	109.5
C14—C13—H13	119.7	O4—C26—H26A	109.5
C12—C13—H13	119.7	O4—C26—H26B	109.5
C13—C14—C9	120.39 (12)	H26A—C26—H26B	109.5
C13—C14—H14	119.8	O4—C26—H26C	109.5
C9—C14—H14	119.8	H26A—C26—H26C	109.5
C16—C15—C12	177.95 (14)	H26B—C26—H26C	109.5
C15—C16—C17	177.90 (14)	C1—O1—C23	118.13 (10)
C22—C17—C18	120.08 (11)	C3—O2—C24	118.91 (10)
C22—C17—C16	119.31 (12)	C19—O3—C25	117.90 (10)
C18—C17—C16	120.60 (11)	C21—O4—C26	118.72 (11)
O1—C1—C2—C3	177.69 (11)	C8—C9—C14—C13	−179.92 (12)
C6—C1—C2—C3	0.59 (18)	C22—C17—C18—C19	0.2 (2)
C1—C2—C3—O2	179.60 (11)	C16—C17—C18—C19	179.07 (12)
C1—C2—C3—C4	−0.90 (18)	C17—C18—C19—O3	−178.99 (12)
O2—C3—C4—C5	179.63 (11)	C17—C18—C19—C20	0.8 (2)
C2—C3—C4—C5	0.08 (18)	O3—C19—C20—C21	178.44 (12)

C3—C4—C5—C6	1.06 (18)	C18—C19—C20—C21	−1.4 (2)
C3—C4—C5—C7	−176.30 (11)	C19—C20—C21—O4	−178.72 (13)
O1—C1—C6—C5	−176.80 (11)	C19—C20—C21—C22	0.9 (2)
C2—C1—C6—C5	0.53 (19)	O4—C21—C22—C17	179.75 (12)
C4—C5—C6—C1	−1.36 (18)	C20—C21—C22—C17	0.1 (2)
C7—C5—C6—C1	175.90 (11)	C18—C17—C22—C21	−0.6 (2)
C14—C9—C10—C11	−0.84 (19)	C16—C17—C22—C21	−179.55 (12)
C8—C9—C10—C11	179.30 (12)	C6—C1—O1—C23	−179.78 (12)
C9—C10—C11—C12	0.59 (19)	C2—C1—O1—C23	2.94 (18)
C10—C11—C12—C13	0.28 (19)	C4—C3—O2—C24	−175.99 (12)
C10—C11—C12—C15	−179.69 (12)	C2—C3—O2—C24	3.55 (18)
C11—C12—C13—C14	−0.90 (19)	C20—C19—O3—C25	−1.8 (2)
C15—C12—C13—C14	179.07 (12)	C18—C19—O3—C25	178.03 (12)
C12—C13—C14—C9	0.65 (19)	C22—C21—O4—C26	179.71 (14)
C10—C9—C14—C13	0.22 (19)	C20—C21—O4—C26	−0.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O4^{i}	0.95	2.42	3.3511 (17)	167
C14—H14···O2^{ii}	0.95	2.37	3.2758 (16)	160

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

Fig. 1

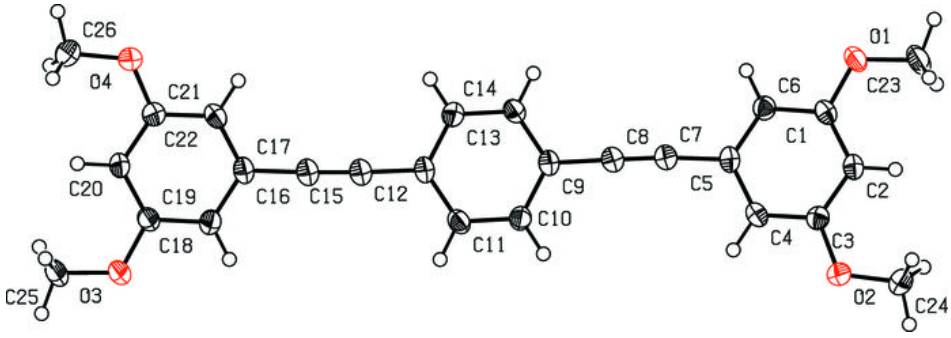
C26
O4
C21
C22
C17
C20
C19
C16
C15
C12
C18
O3
C25
C14
C13
C8
C7
C9
C10
C11
C5
C6
C1
O1
C23
C2
C4
C3
O2
C24

Fig. 2

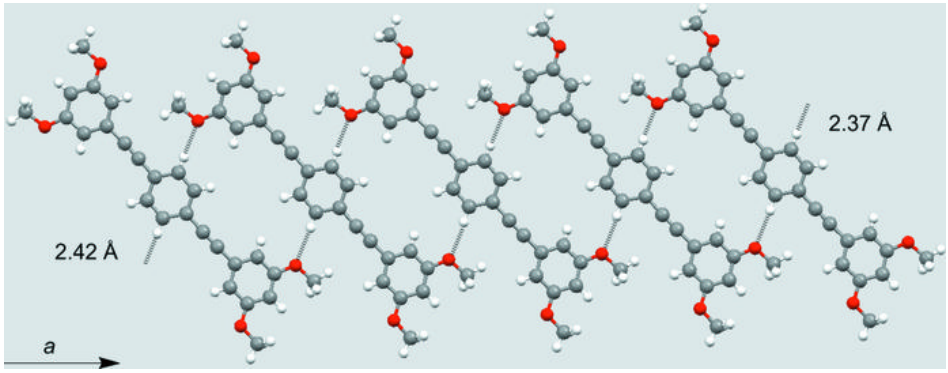

Fig. 3