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1,4-Bis(2-phenylethoxy)benzene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.131
Data-to-parameter ratio = 20.0

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

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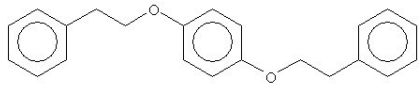
The title compound, $C_{22}H_{22}O_2$, crystallizes in the space group $P2_1/c$, with one half molecule in the asymmetric unit and $Z = 2$.

Comment

The title compound, (I), is a new compound, synthesized as a precursor of substituted phenylene–vinylene oligomers, which are novel compounds for use as semiconductors in an electronic nose (Vanneste *et al.*, 1998; De Wit *et al.*, 1998). The molecule sits on a centre of symmetry. The structure of (I) is, apart from the outer phenyl rings, planar, with a maximum deviation in the torsion angles of −176.74 (13)° for C1—O1—C4—C5. The dihedral angle between the least-squares planes through the central and each of the phenyl rings is 79.38 (9)°. The particular arrangement of the rings allows an intermolecular interaction between the π-system of the outer rings and one of the H atoms of the central ring [$Cg1\cdots H2^{1}$ 2.71 Å; $Cg1$ is the centroid of ring C6–C11; symmetry code: (i) $1-x, \frac{1}{2}-y, \frac{1}{2}+z$]. Other than that, the structure contains no unusual features.



(I)

Experimental

The synthesis of (I) was carried out under a nitrogen atmosphere. Sodium (13.8 g, 0.60 mol) in ethanol (100 ml) was added dropwise to a stirred solution of hydroquinone (33.0 g, 0.30 mol) in ethanol (100 ml). 2-Bromoethylbenzene (84.6 ml, 0.62 mol) was added dropwise to the reaction mixture, which was stirred overnight at room temperature. The temperature was subsequently raised to 318 K for a duration of 7 h, and finally to 353 K overnight. The solvent was evaporated on a rotary evaporator and the resulting oil dissolved in 50 ml of diethyl ether. The ether fraction was washed three times with 50 ml of a 10% NaOH solution and three times with 30 ml of water. After the solution was dried over $MgSO_4$, the solvent was distilled off. After cooling, the resulting oil solidified. Recrystallization from ethanol yielded 11.6 g of 1,4-bis(2-phenylethoxy)benzene, which

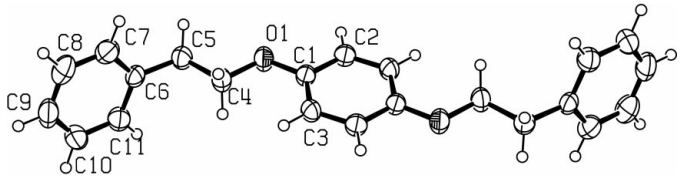


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids; the atom-numbering scheme of the asymmetric unit is shown.

crystallized as white needles. The final yield was 13%. M.p. 335 K; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.32–7.18 (10H, *m*, H7, H11, H9, H8, H10), 6.80 (4H, *s*, H2, H3), 4.10 (2H, *t*, J = 7.17 Hz, H41, H42), 3.05 (2H, *t*, J = 7.10 Hz, H51, H52); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 153.10 (C1), 138.38 (C6), 128.94 (C7, C11), 128.43 (C8, C10), 126.39 (C9), 115.63 (C2), 69.42 (C4), 35.93 (C5).

Crystal data

$C_{22}H_{22}O_2$
M_r = 318.40
Monoclinic, $P2_1/c$
a = 8.9286 (17) Å
b = 11.3470 (11) Å
c = 8.925 (2) Å
β = 103.311 (16)°
V = 879.9 (3) Å^3
Z = 2
D_x = 1.202 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5–16°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colourless
0.3 × 0.3 × 0.2 mm

Data collection

Enraf–Nonius MACH3 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: none
6278 measured reflections
3053 independent reflections
1318 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 32.0°
$h = -13 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = 0 \rightarrow 13$
3 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.131
S = 0.99
3053 reflections
153 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

The low proportion of 'observed' reflections is due to the high temperature movement of the atoms at room temperature, causing the average reflection between 28 and 32° to have an $I/\sigma(I)$ of only 1.53.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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