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1,2-Dimethyl-4,5-bis(phenoxymethyl)benzene

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The molecule of the title compound, $C_{22}H_{22}O_2$, possesses a crystallographically imposed twofold axis. The two terminal phenyl rings both make a dihedral angle of 82.5 (2)° with the central benzene ring. The crystal packing is stabilized mainly by van der Waals forces.

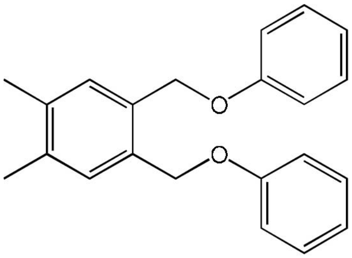
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 17.7

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

Comment

The title compound, (I), is a precursor to substituted phenylene–vinylene oligomers, which are novel compounds for use as semiconductors in an electronic nose (Vanneste *et al.*, 1998).



(I)

The molecule of (I) possesses a crystallographically imposed twofold axis (Fig. 1). The bond lengths and angles are within normal ranges (Table 1) (Allen *et al.*, 1987). The torsion angles C3—C4—C5—O1 and C4—C5—O1—C6 are 90.40 (15) and 178.23 (11)°, respectively. The two terminal phenyl rings both make dihedral angles of 82.5 (2)° with the central benzene ring, while the dihedral angle between the phenyl rings is 56.8 (1)°.

The crystal packing (Fig. 2) is stabilized mainly by van der Waals forces.

Experimental

Sodium hydride (0.48 g, 20 mmol) was added to a stirred solution of 1,2-bis-chloromethyl-4,5-dimethylbenzene (2.03 g, 10 mmol) in anhydrous tetrahydrofuran (THF, 30 ml) under a nitrogen atmosphere. To this mixture, a solution of phenol (1.88 g, 20 mmol) in anhydrous THF (10 ml) was added dropwise and stirred overnight at room temperature. The THF was removed and water was added to it, followed by extraction with dichloromethane. The solvent was evaporated to dryness and the compound was purified by column chromatography to obtain the title compound (yield 2.86 g, 90%). A sample was dissolved in a mixture of hexane–EtOAc (1:6) at room temperature and ambient pressure, and crystals of (I) grew over a period of a week when the solution was exposed to the air.

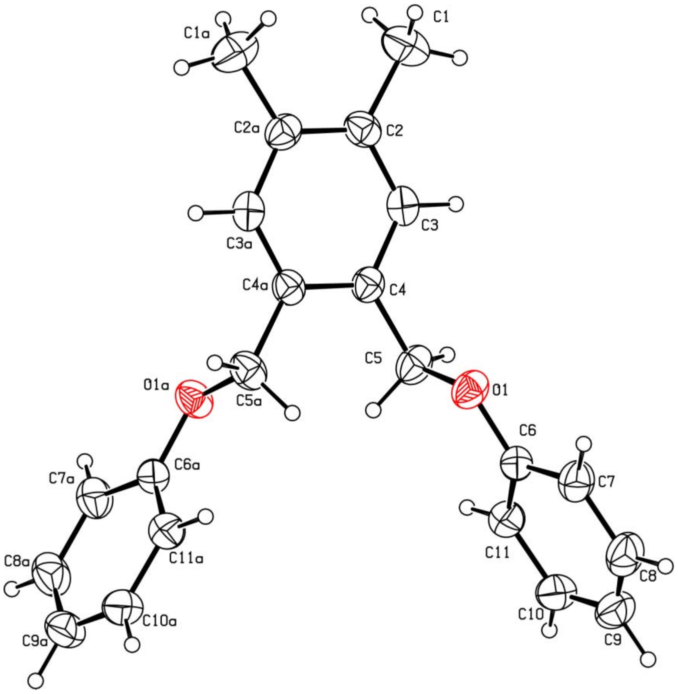


Figure 1
A view of (I), showing the atom-labelling scheme [symmetry code: (a) $1 - x, y, \frac{1}{2} - z$]. Displacement ellipsoids are drawn at the 50% probability level.

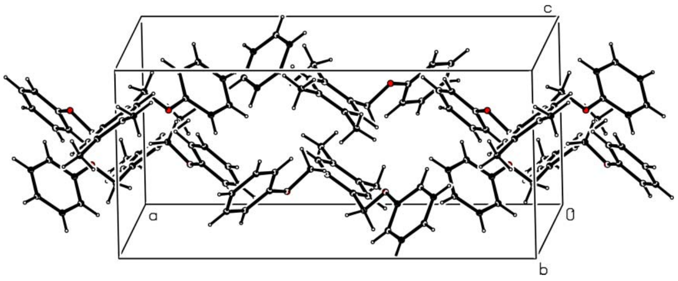


Figure 2
The crystal packing, viewed approximately along the b axis.

Crystal data

$C_{22}H_{22}O_2$
$M_r = 318.40$
Orthorhombic, *Pbcn*
$a = 18.476$ (4) Å
$b = 11.494$ (2) Å
$c = 8.4632$ (17) Å
$V = 1797.2$ (6) Å^3
$Z = 4$
$D_x = 1.177$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 1978 reflections
$\theta = 2.4$–21.6°
$\mu = 0.07$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
11066 measured reflections
1964 independent reflections

1180 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.057$
$\theta_{\rm max} = 27.0°$
$h = -15 \rightarrow 23$
$k = -14 \rightarrow 14$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.120$
$S = 0.89$
1964 reflections
111 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.065P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.14$ e Å^{-3}
Extinction correction: *SHELX97* (Sheldrick, 1997)
Extinction coefficient: 0.0048 (13)

Table 1
Selected geometric parameters (Å, °).

C4—C5	1.5011 (18)	C6—O1	1.3746 (16)
C5—O1	1.4329 (16)		
C3—C4—C5	119.76 (13)	O1—C6—C7	115.68 (13)
O1—C5—C4	108.42 (11)	C6—O1—C5	116.84 (10)

After their location in a difference Fourier map, H atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2–1.5 $U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELX97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, S1–S19.
Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Vanneste, E., De Wit, M., Eyckmans, K. & Geise, H. J. (1998). *Semin. Food Anal.* **3**, 107–113.

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