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1,4-Bis(hexyloxy)benzene

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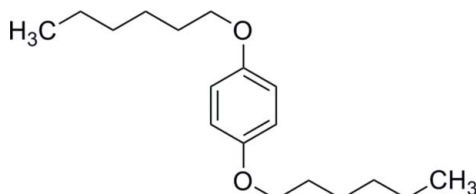
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.067; wR factor = 0.238; data-to-parameter ratio = 16.9.

The asymmetric unit of the title compound, $\text{C}_{18}\text{H}_{30}\text{O}_2$, contains one half-molecule situated on an inversion center. The alkyl chain adopts a fully extended all-*trans* conformation. The C atoms of the alkyl chain are almost coplanar, with a maximum deviation of 0.042 (6) Å from the mean plane, which is inclined to the central benzene ring by 6.80 (9)°. The crystal packing exhibits no short intermolecular contacts.

Related literature

For the synthesis and applications of the title compound, see: Ramesh & Thomas (2010); Mayor & Didschies (2003); Choi *et al.* (2006). For the crystal structures of related compounds, see: Li *et al.* (2008); Thevenet *et al.* (2010).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{30}\text{O}_2$	$V = 896.9$ (11) Å ³
$M_r = 278.42$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.853$ (12) Å	$\mu = 0.07$ mm ⁻¹
$b = 7.512$ (5) Å	$T = 298$ K
$c = 6.364$ (4) Å	$0.06 \times 0.05 \times 0.04$ mm
$\beta = 95.674$ (10)°	

Data collection

Bruker APEXII CCD diffractometer	6024 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	1552 independent reflections
$T_{\min} = 0.996$, $T_{\max} = 0.997$	760 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.099$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$	92 parameters
$wR(F^2) = 0.238$	H-atom parameters constrained
$S = 0.99$	$\Delta\rho_{\text{max}} = 0.17$ e Å ⁻³
1552 reflections	$\Delta\rho_{\text{min}} = -0.15$ e Å ⁻³

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5434).

References

- Bruker (2001). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Choi, K. M., Kim, H. L. & Suh, D. H. (2006). *J. Appl. Polym. Sci.* **101**, 1228–1233.
- Li, Y.-F., Xu, C., Cen, F.-F., Wang, Z.-Q. & Zhang, Y.-Q. (2008). *Acta Cryst.* **E64**, o1930.
- Mayor, M. & Didschies, C. (2003). *Angew. Chem. Int. Ed.* **42**, 3176–3179.
- Ramesh, A. R. & Thomas, K. G. (2010). *Chem. Commun.* **46**, 3457–3459.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Thevenet, D., Neier, R., Sereda, O., Neels, A. & Stoeckli-Evans, H. (2010). *Acta Cryst.* **E66**, o837–o838.

supporting information

Acta Cryst. (2013). E69, o1721 [doi:10.1107/S1600536813029024]

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S1. Comment

The title compound is an important intermediate in the synthesis of conjugated polymers (Mayor & Didschies, 2003; Choi *et al.*, 2006) and supramolecular networks (Ramesh & Thomas, 2010). Herein we report its crystal structure.

In the molecule (Fig. 1), the alkyl chain adopts a fully extended all-*trans* conformation. The C-atoms of the alkyl chain are almost coplanar with the maximum deviation of 0.042 (6) Å from the mean plane, and this mean plane is inclined to the central benzene ring by 6.80 (9)°. The crystal packing exhibits no short intermolecular contacts.

S2. Experimental

The title compound was synthesized according to the known method (Ramesh & Thomas, 2010). Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of the solution in hexane-MeOH (5:1).

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, allowing for free rotation of the methyl groups. The constraint $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ or $1.5 U_{\text{eq}}(\text{C})$ (methyl C) was applied.

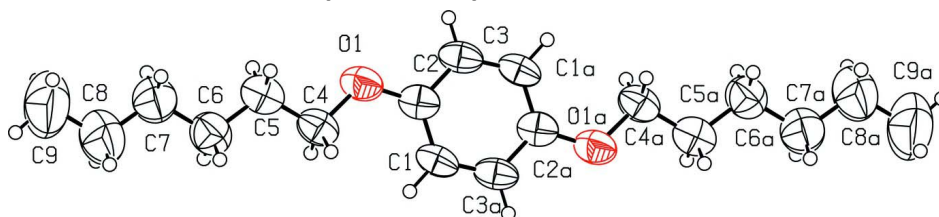


Figure 1

The title molecule with the atom-numbering scheme and 50% probability displacement ellipsoids [symmetry code: (a) $-x, 1 -y, 2 -z$].

1,4-Bis(hexyloxy)benzene

Crystal data

$\text{C}_{18}\text{H}_{30}\text{O}_2$
 $M_r = 278.42$
 Monoclinic, $P2_1/c$
 Hall symbol: $-P 2_1/c$
 $a = 18.853$ (12) Å
 $b = 7.512$ (5) Å
 $c = 6.364$ (4) Å
 $\beta = 95.674$ (10)°
 $V = 896.9$ (11) Å³
 $Z = 2$

$F(000) = 308$
 $D_x = 1.031$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 885 reflections
 $\theta = 2.2$ – 21.8 °
 $\mu = 0.07$ mm⁻¹
 $T = 298$ K
 Block, colourless
 $0.06 \times 0.05 \times 0.04$ mm

Data collection

Bruker APEXII CCD diffractometer	6024 measured reflections
Radiation source: fine-focus sealed tube	1552 independent reflections
Graphite monochromator	760 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.099$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.996$, $T_{\text{max}} = 0.997$	$h = -22 \rightarrow 21$
	$k = -8 \rightarrow 8$
	$l = -7 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.238$	$w = 1/[\sigma^2(F_o^2) + (0.1237P)^2]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
1552 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
92 parameters	$\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.15 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.01445 (17)	0.4133 (3)	0.8176 (4)	0.0693 (9)
H1	0.0241	0.3542	0.6952	0.083*
C2	0.06718 (16)	0.5102 (3)	0.9318 (4)	0.0664 (8)
C3	0.05200 (17)	0.5954 (4)	1.1147 (4)	0.0700 (8)
H3	0.0876	0.6597	1.1928	0.084*
C4	0.15191 (16)	0.4640 (4)	0.6777 (4)	0.0795 (9)
H4A	0.1171	0.5055	0.5661	0.095*
H4B	0.1514	0.3348	0.6782	0.095*
C5	0.22423 (18)	0.5306 (5)	0.6427 (5)	0.0905 (10)
H5A	0.2228	0.6595	0.6360	0.109*
H5B	0.2571	0.4978	0.7634	0.109*
C6	0.25233 (18)	0.4623 (5)	0.4483 (5)	0.0959 (11)
H6A	0.2207	0.4996	0.3269	0.115*
H6B	0.2520	0.3332	0.4520	0.115*
C7	0.3266 (2)	0.5246 (5)	0.4201 (6)	0.1107 (13)
H7A	0.3262	0.6535	0.4098	0.133*

H7B	0.3576	0.4929	0.5452	0.133*
C8	0.3570 (3)	0.4521 (8)	0.2347 (7)	0.1542 (19)
H8A	0.3263	0.4849	0.1095	0.185*
H8B	0.3569	0.3232	0.2443	0.185*
C9	0.4300 (3)	0.5113 (10)	0.2076 (9)	0.202 (3)
H9A	0.4313	0.6389	0.2018	0.303*
H9B	0.4444	0.4631	0.0787	0.303*
H9C	0.4619	0.4704	0.3245	0.303*
O1	0.13529 (11)	0.5307 (3)	0.8769 (3)	0.0818 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.106 (2)	0.0549 (16)	0.0456 (15)	−0.0004 (15)	0.0022 (15)	−0.0034 (12)
C2	0.089 (2)	0.0570 (17)	0.0516 (15)	−0.0033 (13)	−0.0020 (13)	0.0104 (13)
C3	0.103 (2)	0.0531 (16)	0.0516 (15)	−0.0086 (14)	−0.0060 (13)	0.0021 (12)
C4	0.099 (2)	0.0787 (19)	0.0600 (18)	0.0063 (16)	0.0020 (14)	−0.0041 (15)
C5	0.105 (2)	0.085 (2)	0.081 (2)	0.0025 (18)	0.0044 (16)	−0.0080 (17)
C6	0.100 (3)	0.102 (3)	0.086 (2)	0.0084 (19)	0.0097 (17)	−0.0030 (19)
C7	0.108 (3)	0.116 (3)	0.108 (3)	0.002 (2)	0.013 (2)	−0.002 (2)
C8	0.140 (4)	0.200 (5)	0.127 (4)	0.002 (4)	0.041 (3)	−0.017 (4)
C9	0.140 (4)	0.272 (9)	0.205 (6)	−0.003 (4)	0.070 (4)	−0.004 (5)
O1	0.0997 (16)	0.0855 (15)	0.0591 (12)	−0.0089 (11)	0.0017 (10)	−0.0092 (10)

Geometric parameters (Å, °)

C1—C3 ⁱ	1.366 (4)	C5—H5B	0.9700
C1—C2	1.380 (4)	C6—C7	1.505 (5)
C1—H1	0.9300	C6—H6A	0.9700
C2—O1	1.372 (3)	C6—H6B	0.9700
C2—C3	1.383 (4)	C7—C8	1.467 (5)
C3—C1 ⁱ	1.366 (4)	C7—H7A	0.9700
C3—H3	0.9300	C7—H7B	0.9700
C4—O1	1.427 (3)	C8—C9	1.472 (6)
C4—C5	1.490 (4)	C8—H8A	0.9700
C4—H4A	0.9700	C8—H8B	0.9700
C4—H4B	0.9700	C9—H9A	0.9600
C5—C6	1.484 (4)	C9—H9B	0.9600
C5—H5A	0.9700	C9—H9C	0.9600
C3 ⁱ —C1—C2	119.7 (3)	C7—C6—H6A	108.8
C3 ⁱ —C1—H1	120.2	C5—C6—H6B	108.8
C2—C1—H1	120.2	C7—C6—H6B	108.8
O1—C2—C1	124.7 (3)	H6A—C6—H6B	107.7
O1—C2—C3	116.0 (2)	C8—C7—C6	115.0 (4)
C1—C2—C3	119.3 (3)	C8—C7—H7A	108.5
C1 ⁱ —C3—C2	121.1 (2)	C6—C7—H7A	108.5
C1 ⁱ —C3—H3	119.5	C8—C7—H7B	108.5

C2—C3—H3	119.5	C6—C7—H7B	108.5
O1—C4—C5	107.4 (3)	H7A—C7—H7B	107.5
O1—C4—H4A	110.2	C7—C8—C9	115.2 (5)
C5—C4—H4A	110.2	C7—C8—H8A	108.5
O1—C4—H4B	110.2	C9—C8—H8A	108.5
C5—C4—H4B	110.2	C7—C8—H8B	108.5
H4A—C4—H4B	108.5	C9—C8—H8B	108.5
C6—C5—C4	114.6 (3)	H8A—C8—H8B	107.5
C6—C5—H5A	108.6	C8—C9—H9A	109.5
C4—C5—H5A	108.6	C8—C9—H9B	109.5
C6—C5—H5B	108.6	H9A—C9—H9B	109.5
C4—C5—H5B	108.6	C8—C9—H9C	109.5
H5A—C5—H5B	107.6	H9A—C9—H9C	109.5
C5—C6—C7	113.9 (3)	H9B—C9—H9C	109.5
C5—C6—H6A	108.8	C2—O1—C4	118.7 (2)
C3 ⁱ —C1—C2—O1	-178.8 (2)	C5—C6—C7—C8	177.1 (4)
C3 ⁱ —C1—C2—C3	0.7 (4)	C6—C7—C8—C9	-179.4 (4)
O1—C2—C3—C1 ⁱ	178.9 (2)	C1—C2—O1—C4	6.9 (4)
C1—C2—C3—C1 ⁱ	-0.7 (4)	C3—C2—O1—C4	-172.7 (2)
O1—C4—C5—C6	175.7 (2)	C5—C4—O1—C2	170.4 (2)
C4—C5—C6—C7	-177.6 (3)		

Symmetry code: (i) $-x, -y+1, -z+2$.