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1,4-Bis(4-nitrophenoxy)butane

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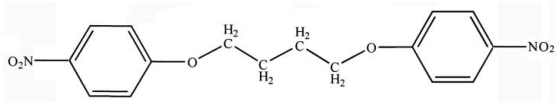
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.134; data-to-parameter ratio = 12.8.

In the crystal structure of the title compound, $C_{16}H_{16}N_2O_6$, the molecule is centrosymmetric. The two benzene rings are linked by a diether strand, forming a non-coplanar structure with a dihedral angle of 5.18 (12)° between the benzene ring and the central chain. The molecular packing is controlled by C—H···π interactions and π–π stacking, with a $Cg1\cdots Cg1(1-x, 1-y, 1-z)$ distance of 3.7687 (12) Å ($Cg1$ is the centroid of the benzene ring).

Related literature

For related literature, see: Day & Arnold (2000); Day *et al.* (2002); Freeman *et al.* (1981); Kim *et al.* (2000).



Experimental

Crystal data

$C_{16}H_{16}N_2O_6$
M_r = 332.31
Monoclinic, $P2_1/n$
a = 7.1273 (5) Å
b = 8.7534 (7) Å
c = 12.8912 (10) Å
β = 99.516 (6)°
V = 793.19 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.23 × 0.16 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.976, T_{max} = 0.988
5846 measured reflections
1408 independent reflections
1043 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.134
S = 1.09
1408 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

$Cg1$ is the centroid of the C1—C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7B···$Cg1^{i}$	0.97	2.97	3.801 (2)	144

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: AT2492).

References

Bruker (2002). *SMART* and *SAINT*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Bruker (2005). *SADABS*. Version 1.22. Bruker AXS, Inc., Madison, Wisconsin, USA.
Day, A. I. & Arnold, A. P. (2000). World Patent WO 0068232.
Day, A. I., Blanch, R. J., Arnold, A. P., Lorenzo, S., Lewis, G. R. & Dance, I. (2002). *Angew. Chem. Int. Ed.* **41**, 275–277.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Freeman, W. A., Mock, W. L. & Shih, N. Y. (1981). *J. Am. Chem. Soc.* **103**, 7367–7368.
Kim, J., Jung, I.-S., Kim, S.-Y., Lee, E., Kang, J.-K., Sakamoto, S., Yamaguchi, K. & Kim, K. (2000). *J. Am. Chem. Soc.* **122**, 540–541.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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1,4-Bis(4-nitrophenoxy)butane

Q.-L. Zhang, Y.-C. Zhao, Y.-Q. Zhang, S.-F. Xue and Z. Tao

Comment

As part of our ongoing investigation on bibenzene compounds, we present a compound(I) containing multiple functional groups that can develop strong intermolecular interactions with cucurbit[*n*]urils (CB[*n*]) (Freeman *et al.*, 1981; Day & Arnold, 2000; Day *et al.*, 2002; Kim *et al.*, 2000).

The crystal structure of the title compound (I) is shown in Fig.1. The molecular is centro-symmetric, the middle point of the C8—C8^{i} bond is located on an inversion center [symmetry code: (i) −*x*, −*y*, −*z* + 1]. The two parallel phenyl rings were linked by ethereal chain forming a non-coplanar structure. The molecules arranges in a step shape like by C—H···π intermolecular π–π stacking between adjacent pyridine rings, with the C7—H7B···*Cg*1^{ii} angle of 144.30 °, H7B···*Cg*1^{ii} distance of 2.9713 Å, C7···*Cg*1^{ii} distances of 3.801 (2) Å, and *Cg*1···*Cg*1^{iii} distances of 3.7687 (12) Å. *Cg*1 is the centroid of the C1–C6-benzene ring [symmetry codes: (ii) 1/2 − *x*, −1/2 + *y*, 1/2 − *z*, (iii) 1 − *x*, 1 − *y*, 1 − *z*].

Experimental

p-toluenesulfonyl chloride (7.62 g, 40 mmol) was added slowly, whilst stirring, to a pyridine solution (50 ml) containing 1,4-butadinol (1.8 g, 20 mmol). The mixture was stirred for about 4 h in the range of 268 K − 278 K. Water(40 ml) was added to the resulting solution, the precipitate was collected by filtration, the solid product was crystallized using ethanol. The solid product (6.85 g, 20 mmol) dissolved in DMF (100 ml) containing K_2CO_3 (2 g), *p*-nitrophenol (0.54 g, 4 mmol) was added slowly, to the DMF (100 ml) solution, and the mixture was heated at 353 K for 24 h, and then the solvent was removed into water and filtered, the residue was washed with water. The solid product was dissolved in 40 ml e thanol. Single crystals of (I) were obtained after three days.

Refinement

All H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

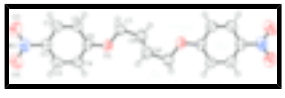

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) −*x*, −*y*, −*z* + 1].

1,4-Bis(4-nitrophenoxy)butane

Crystal data

$C_{16}H_{16}N_2O_6$ F_{000} = 348

M_r = 332.31	D_x = 1.391 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1408 reflections
a = 7.1273 (5) Å	θ = 2.8–25.0º
b = 8.7534 (7) Å	μ = 0.11 mm^{-1}
c = 12.8912 (10) Å	T = 293 (2) K
β = 99.516 (6)º	Prism, colourless
V = 793.19 (10) Å^3	0.23 × 0.16 × 0.11 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	1408 independent reflections
Radiation source: fine-focus sealed tube	1043 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -8 \rightarrow 8$
T_{min} = 0.976, T_{max} = 0.988	$k = -10 \rightarrow 10$
5846 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.1309P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.134	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
1408 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
110 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.014 (4)
Secondary atom site location: difference Fourier map	

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	0.4995 (3)	0.5527 (2)	0.35002 (14)	0.0519 (5)
C2	0.3176 (3)	0.5840 (2)	0.36693 (16)	0.0589 (6)
H2	0.2749	0.6843	0.3674	0.071*
C3	0.5641 (3)	0.4051 (2)	0.34752 (15)	0.0571 (6)
H3	0.6865	0.3860	0.3346	0.069*
C4	0.2001 (3)	0.4653 (2)	0.38298 (16)	0.0586 (6)
H4	0.0769	0.4853	0.3943	0.070*
C5	0.4468 (3)	0.2852 (2)	0.36426 (15)	0.0537 (5)
H5	0.4900	0.1850	0.3633	0.064*
C6	0.2638 (3)	0.3154 (2)	0.38251 (14)	0.0498 (5)
C7	0.1989 (3)	0.0542 (2)	0.42172 (17)	0.0587 (6)
H7A	0.3053	0.0525	0.4793	0.070*
H7B	0.2388	0.0081	0.3605	0.070*
C8	0.0334 (3)	−0.0313 (3)	0.45115 (16)	0.0636 (6)
H8A	0.0690	−0.1376	0.4631	0.076*
H8B	−0.0714	−0.0273	0.3927	0.076*
N1	0.6235 (3)	0.6788 (2)	0.33313 (15)	0.0683 (6)
O1	0.13674 (19)	0.20758 (17)	0.39908 (11)	0.0630 (5)
O2	0.5651 (3)	0.8097 (2)	0.33911 (15)	0.0893 (6)
O3	0.7805 (3)	0.6492 (2)	0.31313 (18)	0.1070 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0571 (12)	0.0525 (13)	0.0450 (11)	−0.0092 (10)	0.0049 (8)	0.0021 (9)
C2	0.0711 (14)	0.0473 (13)	0.0580 (12)	0.0057 (10)	0.0101 (10)	0.0030 (9)
C3	0.0487 (11)	0.0647 (15)	0.0593 (13)	−0.0031 (10)	0.0127 (9)	−0.0019 (10)
C4	0.0556 (12)	0.0603 (14)	0.0627 (12)	0.0055 (11)	0.0185 (9)	0.0058 (11)
C5	0.0553 (12)	0.0481 (12)	0.0596 (12)	−0.0014 (10)	0.0151 (9)	−0.0006 (10)
C6	0.0530 (11)	0.0541 (13)	0.0437 (10)	−0.0047 (9)	0.0123 (8)	0.0048 (9)
C7	0.0695 (13)	0.0519 (14)	0.0573 (12)	−0.0054 (10)	0.0179 (10)	0.0012 (10)
C8	0.0812 (15)	0.0584 (14)	0.0553 (12)	−0.0180 (12)	0.0231 (10)	−0.0042 (10)
N1	0.0707 (13)	0.0611 (14)	0.0703 (12)	−0.0118 (10)	0.0036 (10)	0.0042 (10)
O1	0.0562 (9)	0.0590 (10)	0.0767 (10)	−0.0052 (7)	0.0196 (7)	0.0153 (7)
O2	0.0978 (13)	0.0600 (12)	0.1059 (14)	−0.0131 (10)	0.0046 (10)	0.0019 (10)
O3	0.0726 (12)	0.0928 (15)	0.161 (2)	−0.0150 (11)	0.0339 (12)	0.0196 (13)

Geometric parameters (Å, °)

C1—C3	1.374 (3)	C6—O1	1.349 (2)

C1—C2	1.378 (3)	C7—O1	1.429 (2)
C1—N1	1.453 (3)	C7—C8	1.497 (3)
C2—C4	1.372 (3)	C7—H7A	0.9700
C2—H2	0.9300	C7—H7B	0.9700
C3—C5	1.381 (3)	C8—C8^{i}	1.520 (4)
C3—H3	0.9300	C8—H8A	0.9700
C4—C6	1.389 (3)	C8—H8B	0.9700
C4—H4	0.9300	N1—O3	1.217 (3)
C5—C6	1.388 (3)	N1—O2	1.226 (3)
C5—H5	0.9300		
C3—C1—C2	121.23 (19)	C5—C6—C4	119.86 (18)
C3—C1—N1	119.76 (19)	O1—C7—C8	106.91 (17)
C2—C1—N1	119.0 (2)	O1—C7—H7A	110.3
C4—C2—C1	119.2 (2)	C8—C7—H7A	110.3
C4—C2—H2	120.4	O1—C7—H7B	110.3
C1—C2—H2	120.4	C8—C7—H7B	110.3
C1—C3—C5	119.82 (19)	H7A—C7—H7B	108.6
C1—C3—H3	120.1	C7—C8—C8^{i}	113.4 (2)
C5—C3—H3	120.1	C7—C8—H8A	108.9
C2—C4—C6	120.44 (19)	C8^{i}—C8—H8A	108.9
C2—C4—H4	119.8	C7—C8—H8B	108.9
C6—C4—H4	119.8	C8^{i}—C8—H8B	108.9
C3—C5—C6	119.44 (19)	H8A—C8—H8B	107.7
C3—C5—H5	120.3	O3—N1—O2	123.1 (2)
C6—C5—H5	120.3	O3—N1—C1	118.3 (2)
O1—C6—C5	124.59 (19)	O2—N1—C1	118.6 (2)
O1—C6—C4	115.54 (17)	C6—O1—C7	119.74 (16)
C3—C1—C2—C4	0.9 (3)	C2—C4—C6—C5	−0.9 (3)
N1—C1—C2—C4	−179.95 (18)	O1—C7—C8—C8^{i}	−61.9 (3)
C2—C1—C3—C5	−1.3 (3)	C3—C1—N1—O3	2.7 (3)
N1—C1—C3—C5	179.57 (18)	C2—C1—N1—O3	−176.4 (2)
C1—C2—C4—C6	0.2 (3)	C3—C1—N1—O2	−177.66 (19)
C1—C3—C5—C6	0.6 (3)	C2—C1—N1—O2	3.2 (3)
C3—C5—C6—O1	179.52 (18)	C5—C6—O1—C7	13.9 (3)
C3—C5—C6—C4	0.5 (3)	C4—C6—O1—C7	−167.07 (17)
C2—C4—C6—O1	180.00 (18)	C8—C7—O1—C6	172.01 (17)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7B···Cg1^{ii}	0.97	2.97	3.801 (2)	144

Symmetry codes: (ii) −*x*+1/2, *y*−1/2, −*z*+1/2.
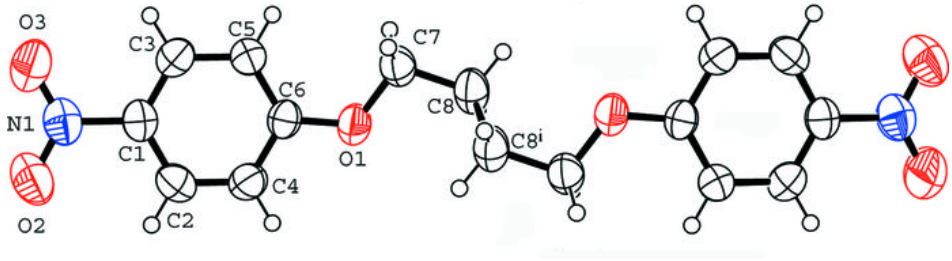
Fig. 1