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1,10-Bis(2-aminophenoxy)decane

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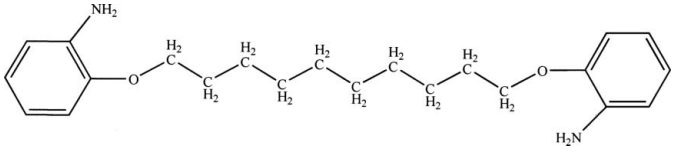
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.134; data-to-parameter ratio = 15.5.

The crystal structure of the title compound, $C_{22}H_{32}N_2O_2$, contains two independent molecules, each of which is centrosymmetric. Each molecule, with benzene rings linked by a diether strand, is essentially planar except for H atoms. There are two N—H···O and one N—H···N hydrogen bonds. The molecular packing is also controlled by N—H···π and C—H···π interactions.

Related literature

For related literature, see: Lacroix (2001); Sabater *et al.* (2001).



Experimental

Crystal data

$C_{22}H_{32}N_2O_2$
M_r = 356.50
Triclinic, $P\overline{1}$
a = 6.0138 (9) Å
b = 7.1653 (10) Å
c = 25.932 (4) Å
α = 84.666 (6)°
β = 88.774 (7)°
γ = 71.078 (4)°
V = 1052.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.18 × 0.13 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.987, T_{max} = 0.993
11351 measured reflections
3651 independent reflections
2303 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.06
3651 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C12–C17 benzene rings.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.86	2.47	3.300 (3)	163
N1—H1B···O1	0.86	2.30	2.630 (2)	103
N2—H2B···O2	0.86	2.28	2.618 (2)	103
N1—H1A···$Cg2^{i}$	0.86	2.58	3.436 (2)	175
C7—H7A···$Cg1^{ii}$	0.97	3.07	3.8452 (2)	138
C14—H14A···$Cg1^{iii}$	0.93	3.27	3.966 (2)	134
C21—H21B···$Cg2^{iv}$	0.97	3.29	4.051 (2)	137

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

Data collection: *APEX2* (Bruker, 2005); 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: RK2040).

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supplementary materials

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Q.-L. Zhang, X.-C. Zhu, Y.-Q. Zhang and B.-X. Zhu

Comment

Diamine compounds not only are the materials of preparing dyes, paints, oil dope, but also are the important intermediate of synthesizing Schiff base compounds. Recently, Schiff base metal complexes have been widely investigated for their properties and applications in different fields, such as catalysis (Sabater *et al.*, 2001) and materials chemistry (Lacroix, 2001).

The structure of the title compound $C_{22}H_{32}N_2O_2$ (I) contains two independent molecules, which occupy the center of symmetry positions in the middle of C11—C11*a* and C22—C22*b* bonds, respectively (symmetry codes: (*a*) −*x* + 1,-*y* + 2,-*z* + 1 and (*b*) −*x* + 2,-*y*,-*z*). In the molecular structure of the (I), the two phenyl rings were linked by ethereal chain forming a non–coplanar structure (Fig. 1). The crystal structure displays two N—H···O and one N—H···N hydrogen bonds (see hydroge–bond table). In the crystal structure, N—H···π and C—H···π interactions occur between adjacent molecules, with N1—H1A···*Cg*(2)^{i} angle of 174.99°, H1A···*Cg*(2)^{i} distance of 2.5782 Å, N1···*Cg*(2)^{i} distances of 3.436 (2) Å, C7—H7A···*Cg*(1)^{ii} angle of 137.90°, H7A···*Cg*(1)^{ii} distance of 3.0698 Å, N1···*Cg*(1)^{ii} distances of 3.8452 (2) Å, C14—H14A···*Cg*(1)^{iii} angle of 133.77°, H14A···*Cg*(1)^{iii} distance of 3.2656 Å, C14···*Cg*(1)^{iii} distances of 3.966 (2)Å and C21—H21B···*Cg*(2)^{iv} angle of 136.73°, H21B···*Cg*(2))^{iv} distance of 3.2896 Å, C21···*Cg*(2)^{iv} distances of 4.051 (2) Å, respectively. *Cg*(1)^{i}, *Cg*(1)^{ii}, *Cg*(1)^{iii} and *Cg*(2)^{iv} are the centroid of the C1–C6 benzene and C12—C17 benzene rings (symmetry codes: (i) −*x* + *y*, *y*, *z*; (ii) 1 + *x*, *y*, *z*; (iii) *x*, 1 + *y*, *z*; (iv) 1 + *x*, −1 + *y*, *z*).

Experimental

p–Toluenesulfonyl chloride (7.62 g, 40 mmol) was added slowly, whilst stirring, to a pyridine solution (50 ml) containing 1,10–hexanediol (3.48 g, 20 mmol). The mixture was stirred for about 4 h in the range of 268–278 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 (0.852 g, 2 mmol) dissolved in DMF (100 ml) containing K_2CO_3 (2 g), *o*–hydroxyaniline (0.38 g, 4 mmol) was added slowly, to the DMF solution and the mixture was heated at 353 K for 10 h and then the solvent was removed under reduced pressure. The crude product was purified by column chromatography over silica gel using 80% dichloromethane–hexane to afford pure crystals (I), 0.492 g, a yield of 81%. Single crystals suitable for *X*–ray diffraction were obtained from the 60% C_2H_5OH–CH_2Cl_2 mixture by slow evaporation at room temperature.

Refinement

All H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, N—H = 0.86Å and with U_{iso}(H) = 1.2 U_{eq}(C, N).

Figures

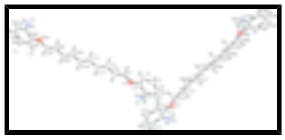


Fig. 1. The molecular structure of (I) with the numbering scheme. Displacement ellipsoids are shown with 30% probability level (symmetry codes:(*a*) −*x* + 1, −*y* + 2, −*z* + 1; (*b*) −*x* + 2, −*y*, −*z*).

1,10-Bis(2-aminophenoxy)decane

Crystal data

$C_{22}H_{32}N_2O_2$	$Z = 2$
$M_r = 356.50$	$F_{000} = 388$
Triclinic, $P\overline{1}$	$D_x = 1.125$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.0138$ (9) Å	Cell parameters from 11351 reflections
$b = 7.1653$ (10) Å	$\theta = 0.8$–25.0º
$c = 25.932$ (4) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 84.666$ (6)º	$T = 293$ (2) K
$\beta = 88.774$ (7)º	Prism, colourless
$\gamma = 71.078$ (4)º	0.18 × 0.13 × 0.08 mm
$V = 1052.4$ (3) Å^3	

Data collection

Bruker APEX II CCD area-detector diffractometer	3651 independent reflections
Radiation source: Fine–focus sealed tube	2303 reflections with $I > 2\sigma(I)$
Monochromator: Graphite	$R_{int} = 0.030$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ– and ω–scan	$\theta_{min} = 0.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -7 \rightarrow 6$
$T_{min} = 0.987$, $T_{max} = 0.993$	$k = -8 \rightarrow 8$
11351 measured reflections	$l = -30 \rightarrow 29$

Refinement

Refinement on F^2	Hydrogen site location: Geom
Least-squares matrix: Full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.0396P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.134$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
3651 reflections	$\Delta\rho_{min} = -0.11$ e Å^{-3}

235 parameters

Primary atom site location: Direct
Secondary atom site location: Difmap

Extinction correction: SHELXL97, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.128

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 $F^2 > 2\sigma(F^2)$ 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	−0.4800 (3)	0.6252 (2)	0.30398 (7)	0.0635 (5)
C2	−0.6094 (3)	0.5138 (3)	0.28764 (7)	0.0712 (5)
H2	−0.7256	0.5696	0.2624	0.085*
C3	−0.5696 (4)	0.3215 (3)	0.30801 (8)	0.0756 (6)
H3	−0.6589	0.2485	0.2967	0.091*
C4	−0.3988 (4)	0.2378 (3)	0.34489 (8)	0.0781 (6)
H4	−0.3713	0.1075	0.3586	0.094*
C5	−0.2663 (3)	0.3465 (3)	0.36198 (7)	0.0719 (5)
H5	−0.1489	0.2888	0.3868	0.086*
C6	−0.3083 (3)	0.5398 (2)	0.34220 (7)	0.0605 (5)
C7	−0.0239 (3)	0.5993 (3)	0.39754 (7)	0.0689 (5)
H7A	0.1087	0.4899	0.3875	0.083*
H7B	−0.0911	0.5554	0.4288	0.083*
C8	0.0530 (3)	0.7731 (3)	0.40642 (7)	0.0718 (5)
H8A	−0.0840	0.8810	0.4153	0.086*
H8B	0.1138	0.8163	0.3742	0.086*
C9	0.2379 (3)	0.7359 (3)	0.44833 (7)	0.0715 (5)
H9A	0.3784	0.6316	0.4393	0.086*
H9B	0.1800	0.6916	0.4808	0.086*
C10	0.2990 (4)	0.9216 (3)	0.45502 (8)	0.0779 (6)
H10A	0.3592	0.9624	0.4224	0.093*
H10B	0.1553	1.0262	0.4622	0.093*
C11	0.4746 (4)	0.9042 (3)	0.49681 (7)	0.0765 (6)
H11A	0.6206	0.8031	0.4892	0.092*
H11B	0.4171	0.8605	0.5294	0.092*
C12	−0.0083 (3)	0.9033 (3)	0.18955 (8)	0.0685 (5)
C13	−0.1008 (4)	1.0721 (3)	0.21528 (8)	0.0787 (6)
H13	−0.2335	1.0855	0.2356	0.094*
C14	−0.0016 (4)	1.2196 (3)	0.21158 (8)	0.0837 (6)

H14	−0.0656	1.3304	0.2298	0.100*
C15	0.1925 (4)	1.2053 (3)	0.18105 (8)	0.0830 (6)
H15	0.2596	1.3059	0.1784	0.100*
C16	0.2869 (4)	1.0378 (3)	0.15426 (7)	0.0780 (6)
H16	0.4174	1.0267	0.1334	0.094*
C17	0.1884 (3)	0.8893 (3)	0.15847 (7)	0.0669 (5)
C18	0.4753 (3)	0.6741 (3)	0.10493 (8)	0.0823 (6)
H18A	0.6034	0.6890	0.1245	0.099*
H18B	0.4489	0.7643	0.0737	0.099*
C19	0.5331 (4)	0.4638 (3)	0.09153 (8)	0.0840 (6)
H19A	0.3967	0.4508	0.0748	0.101*
H19B	0.5623	0.3771	0.1234	0.101*
C20	0.7430 (4)	0.3932 (3)	0.05650 (8)	0.0837 (6)
H20A	0.7179	0.4812	0.0249	0.100*
H20B	0.8823	0.3987	0.0736	0.100*
C21	0.7829 (4)	0.1840 (3)	0.04315 (8)	0.0831 (6)
H21A	0.6402	0.1792	0.0274	0.100*
H21B	0.8104	0.0973	0.0750	0.100*
C22	0.9851 (4)	0.1039 (3)	0.00703 (8)	0.0842 (6)
H22A	1.1292	0.1034	0.0232	0.101*
H22B	0.9607	0.1923	−0.0245	0.101*
N1	−0.5123 (3)	0.8182 (2)	0.28294 (7)	0.0932 (6)
H1A	−0.6158	0.8717	0.2589	0.112*
H1B	−0.4288	0.8838	0.2940	0.112*
N2	−0.1044 (3)	0.7523 (2)	0.19298 (8)	0.0967 (6)
H2A	−0.2266	0.7609	0.2117	0.116*
H2B	−0.0422	0.6495	0.1764	0.116*
O1	−0.1958 (2)	0.66528 (17)	0.35693 (5)	0.0776 (4)
O2	0.2675 (2)	0.71497 (19)	0.13528 (5)	0.0870 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0744 (13)	0.0562 (10)	0.0565 (12)	−0.0163 (9)	−0.0026 (10)	−0.0052 (9)
C2	0.0774 (13)	0.0620 (11)	0.0697 (13)	−0.0150 (10)	−0.0127 (10)	−0.0081 (10)
C3	0.0862 (15)	0.0600 (12)	0.0819 (15)	−0.0226 (10)	−0.0104 (12)	−0.0150 (10)
C4	0.0996 (16)	0.0516 (10)	0.0811 (15)	−0.0210 (11)	−0.0091 (13)	−0.0060 (10)
C5	0.0818 (14)	0.0577 (11)	0.0692 (13)	−0.0127 (10)	−0.0145 (10)	−0.0041 (9)
C6	0.0706 (12)	0.0545 (10)	0.0572 (11)	−0.0199 (9)	−0.0007 (10)	−0.0100 (9)
C7	0.0722 (12)	0.0665 (11)	0.0657 (12)	−0.0174 (9)	−0.0082 (10)	−0.0100 (9)
C8	0.0751 (13)	0.0745 (12)	0.0678 (13)	−0.0258 (10)	−0.0019 (10)	−0.0094 (10)
C9	0.0701 (13)	0.0744 (12)	0.0718 (13)	−0.0232 (10)	−0.0004 (11)	−0.0155 (10)
C10	0.0813 (14)	0.0875 (14)	0.0717 (14)	−0.0357 (11)	−0.0031 (11)	−0.0098 (11)
C11	0.0800 (14)	0.0836 (13)	0.0713 (13)	−0.0314 (11)	0.0019 (11)	−0.0171 (11)
C12	0.0578 (12)	0.0695 (12)	0.0718 (13)	−0.0081 (9)	−0.0058 (10)	−0.0184 (10)
C13	0.0692 (13)	0.0708 (12)	0.0873 (15)	−0.0066 (10)	0.0103 (11)	−0.0233 (11)
C14	0.0916 (16)	0.0645 (12)	0.0877 (16)	−0.0112 (11)	0.0103 (13)	−0.0233 (11)
C15	0.0924 (16)	0.0689 (12)	0.0864 (15)	−0.0219 (11)	0.0094 (13)	−0.0178 (11)

C16	0.0753 (14)	0.0830 (13)	0.0686 (13)	−0.0146 (11)	0.0096 (11)	−0.0135 (11)
C17	0.0633 (12)	0.0667 (11)	0.0614 (12)	−0.0046 (9)	−0.0066 (10)	−0.0180 (9)
C18	0.0674 (13)	0.0959 (15)	0.0747 (14)	−0.0076 (11)	0.0027 (11)	−0.0329 (11)
C19	0.0795 (14)	0.0854 (14)	0.0709 (14)	−0.0004 (11)	0.0080 (11)	−0.0235 (11)
C20	0.0734 (14)	0.0885 (14)	0.0745 (14)	−0.0009 (11)	0.0033 (11)	−0.0260 (11)
C21	0.0785 (14)	0.0827 (13)	0.0691 (14)	0.0022 (11)	0.0077 (11)	−0.0168 (11)
C22	0.0753 (14)	0.0820 (13)	0.0768 (14)	0.0031 (11)	0.0079 (12)	−0.0207 (11)
N1	0.1217 (15)	0.0657 (10)	0.0945 (13)	−0.0383 (10)	−0.0410 (11)	0.0212 (9)
N2	0.0746 (12)	0.0878 (12)	0.1345 (16)	−0.0260 (10)	0.0147 (11)	−0.0475 (11)
O1	0.0927 (10)	0.0660 (8)	0.0765 (9)	−0.0300 (7)	−0.0240 (8)	0.0033 (7)
O2	0.0780 (9)	0.0863 (9)	0.0933 (10)	−0.0135 (7)	0.0158 (8)	−0.0417 (8)

Geometric parameters (Å, °)

C1—C2	1.379 (2)	C12—C17	1.398 (3)
C1—N1	1.392 (2)	C13—C14	1.368 (3)
C1—C6	1.394 (2)	C13—H13	0.9300
C2—C3	1.375 (2)	C14—C15	1.378 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.366 (3)	C15—C16	1.393 (3)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.386 (2)	C16—C17	1.371 (3)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.375 (2)	C17—O2	1.375 (2)
C5—H5	0.9300	C18—O2	1.425 (2)
C6—O1	1.3713 (19)	C18—C19	1.505 (3)
C7—O1	1.428 (2)	C18—H18A	0.9700
C7—C8	1.500 (2)	C18—H18B	0.9700
C7—H7A	0.9700	C19—C20	1.515 (3)
C7—H7B	0.9700	C19—H19A	0.9700
C8—C9	1.515 (2)	C19—H19B	0.9700
C8—H8A	0.9700	C20—C21	1.511 (3)
C8—H8B	0.9700	C20—H20A	0.9700
C9—C10	1.516 (2)	C20—H20B	0.9700
C9—H9A	0.9700	C21—C22	1.511 (3)
C9—H9B	0.9700	C21—H21A	0.9700
C10—C11	1.498 (2)	C21—H21B	0.9700
C10—H10A	0.9700	C22—C22^{ii}	1.518 (4)
C10—H10B	0.9700	C22—H22A	0.9700
C11—C11^{i}	1.523 (3)	C22—H22B	0.9700
C11—H11A	0.9700	N1—H1A	0.8600
C11—H11B	0.9700	N1—H1B	0.8600
C12—N2	1.378 (2)	N2—H2A	0.8600
C12—C13	1.384 (2)	N2—H2B	0.8600
C2—C1—N1	122.20 (18)	C14—C13—H13	119.2
C2—C1—C6	118.71 (16)	C12—C13—H13	119.2
N1—C1—C6	119.08 (16)	C13—C14—C15	120.43 (18)
C3—C2—C1	121.09 (18)	C13—C14—H14	119.8

C3—C2—H2	119.5	C15—C14—H14	119.8
C1—C2—H2	119.5	C14—C15—C16	118.99 (19)
C4—C3—C2	119.90 (18)	C14—C15—H15	120.5
C4—C3—H3	120.0	C16—C15—H15	120.5
C2—C3—H3	120.0	C17—C16—C15	120.4 (2)
C3—C4—C5	120.13 (18)	C17—C16—H16	119.8
C3—C4—H4	119.9	C15—C16—H16	119.8
C5—C4—H4	119.9	C16—C17—O2	126.19 (19)
C6—C5—C4	120.02 (18)	C16—C17—C12	120.68 (17)
C6—C5—H5	120.0	O2—C17—C12	113.11 (17)
C4—C5—H5	120.0	O2—C18—C19	106.50 (17)
O1—C6—C5	125.87 (17)	O2—C18—H18A	110.4
O1—C6—C1	114.00 (15)	C19—C18—H18A	110.4
C5—C6—C1	120.12 (16)	O2—C18—H18B	110.4
O1—C7—C8	106.42 (14)	C19—C18—H18B	110.4
O1—C7—H7A	110.4	H18A—C18—H18B	108.6
C8—C7—H7A	110.4	C18—C19—C20	115.17 (18)
O1—C7—H7B	110.4	C18—C19—H19A	108.5
C8—C7—H7B	110.4	C20—C19—H19A	108.5
H7A—C7—H7B	108.6	C18—C19—H19B	108.5
C7—C8—C9	115.48 (16)	C20—C19—H19B	108.5
C7—C8—H8A	108.4	H19A—C19—H19B	107.5
C9—C8—H8A	108.4	C21—C20—C19	111.83 (18)
C7—C8—H8B	108.4	C21—C20—H20A	109.3
C9—C8—H8B	108.4	C19—C20—H20A	109.3
H8A—C8—H8B	107.5	C21—C20—H20B	109.3
C8—C9—C10	111.26 (16)	C19—C20—H20B	109.3
C8—C9—H9A	109.4	H20A—C20—H20B	107.9
C10—C9—H9A	109.4	C20—C21—C22	115.31 (18)
C8—C9—H9B	109.4	C20—C21—H21A	108.4
C10—C9—H9B	109.4	C22—C21—H21A	108.4
H9A—C9—H9B	108.0	C20—C21—H21B	108.4
C11—C10—C9	115.99 (17)	C22—C21—H21B	108.4
C11—C10—H10A	108.3	H21A—C21—H21B	107.5
C9—C10—H10A	108.3	C21—C22—C22^{ii}	113.9 (2)
C11—C10—H10B	108.3	C21—C22—H22A	108.8
C9—C10—H10B	108.3	C22^{ii}—C22—H22A	108.8
H10A—C10—H10B	107.4	C21—C22—H22B	108.8
C10—C11—C11^{i}	114.2 (2)	C22^{ii}—C22—H22B	108.8
C10—C11—H11A	108.7	H22A—C22—H22B	107.7
C11^{i}—C11—H11A	108.7	C1—N1—H1A	120.0
C10—C11—H11B	108.7	C1—N1—H1B	120.0
C11^{i}—C11—H11B	108.7	H1A—N1—H1B	120.0
H11A—C11—H11B	107.6	C12—N2—H2A	120.0
N2—C12—C13	122.54 (19)	C12—N2—H2B	120.0
N2—C12—C17	119.55 (17)	H2A—N2—H2B	120.0
C13—C12—C17	117.90 (19)	C6—O1—C7	119.66 (13)
C14—C13—C12	121.6 (2)	C17—O2—C18	119.54 (16)

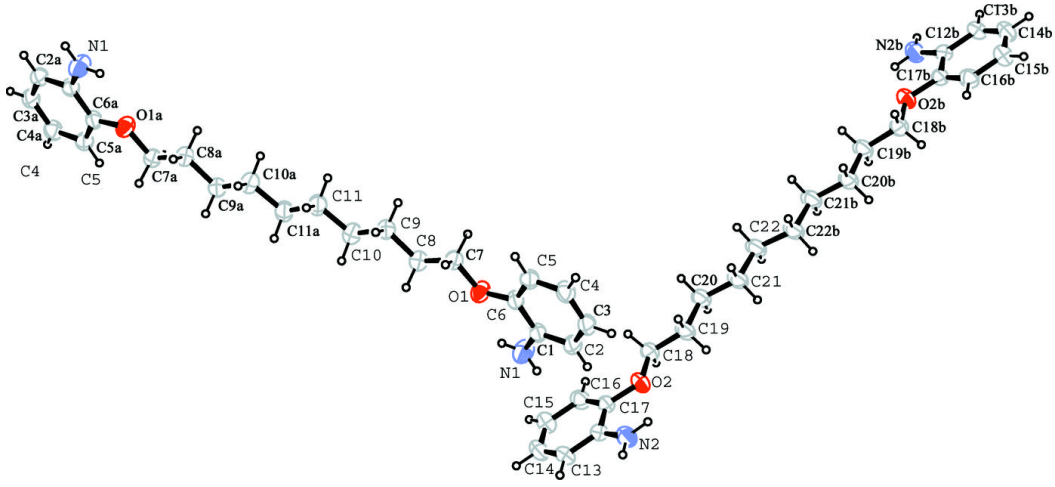
N1—C1—C2—C3	178.13 (19)	C13—C14—C15—C16	−0.4 (3)
C6—C1—C2—C3	−0.7 (3)	C14—C15—C16—C17	−0.3 (3)
C1—C2—C3—C4	−0.3 (3)	C15—C16—C17—O2	−178.22 (17)
C2—C3—C4—C5	0.3 (3)	C15—C16—C17—C12	0.1 (3)
C3—C4—C5—C6	0.7 (3)	N2—C12—C17—C16	179.78 (18)
C4—C5—C6—O1	177.70 (17)	C13—C12—C17—C16	0.7 (3)
C4—C5—C6—C1	−1.7 (3)	N2—C12—C17—O2	−1.7 (3)
C2—C1—C6—O1	−177.78 (16)	C13—C12—C17—O2	179.23 (16)
N1—C1—C6—O1	3.4 (2)	O2—C18—C19—C20	176.78 (17)
C2—C1—C6—C5	1.7 (3)	C18—C19—C20—C21	−177.64 (17)
N1—C1—C6—C5	−177.21 (18)	C19—C20—C21—C22	178.32 (17)
O1—C7—C8—C9	−179.84 (15)	C20—C21—C22—C22^{ii}	−178.0 (2)
C7—C8—C9—C10	−178.70 (16)	C5—C6—O1—C7	−2.4 (3)
C8—C9—C10—C11	177.98 (16)	C1—C6—O1—C7	177.03 (15)
C9—C10—C11—C11^{i}	−178.3 (2)	C8—C7—O1—C6	−176.43 (15)
N2—C12—C13—C14	179.58 (19)	C16—C17—O2—C18	2.3 (3)
C17—C12—C13—C14	−1.3 (3)	C12—C17—O2—C18	−176.21 (17)
C12—C13—C14—C15	1.2 (3)	C19—C18—O2—C17	172.20 (15)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1	0.86	2.47	3.300 (3)	163
N1—H1B···O1	0.86	2.30	2.630 (2)	103
N2—H2B···O2	0.86	2.28	2.618 (2)	103

Fig. 1


N1
C2a
C6a
O1a
C3a
C4a
C4
C5
C5a
C7a
C8a
C9a
C10a
C11a
C11
C10
C9
C8
C7
O1
C6
C5
C4
C3
C2
C1
N1
C18
C19
C20
C21
C22
C22b
C21b
C20b
C19b
C18b
O2b
C17b
C16b
C15b
C14b
C13b
C12b
N2b
C16
O2
C17
C15
C14
C13
N2