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1,3-Bis(2-aminophenoxy)propan-2-ol

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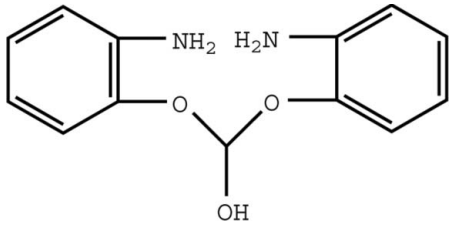
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.146; data-to-parameter ratio = 13.4.

In the structure of the title compound, $C_{15}H_{18}N_2O_3$, the two benzene rings are linked by an ethereal chain, forming a non-coplanar structure. The crystal structure exhibits a layer formation. The structure displays N—H···O, N—H···N and O—H···N hydrogen bonding.

Related literature

For related literature, see: Bella *et al.* (2004); Lacroix (2001); Sabater *et al.* (2001).



Experimental

Crystal data

$C_{15}H_{18}N_2O_3$
M_r = 274.31
Monoclinic, $P2_1/c$
a = 14.069 (2) Å
b = 5.8636 (9) Å
c = 17.112 (3) Å
β = 103.418 (7)°
V = 1373.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.21 × 0.17 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.981, T_{max} = 0.987
9223 measured reflections
2382 independent reflections
1780 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.10
2382 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.24	3.061 (2)	161
N1—H1B···N1^{i}	0.86	2.66	3.353 (4)	139
N2—H2B···O2^{ii}	0.86	2.41	3.125 (2)	142
O2—H2C···N2^{iii}	0.82	2.31	3.125 (2)	173

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

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: AT2269).

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supplementary materials

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1,3-Bis(2-aminophenoxy)propan-2-ol

Z.-Y. Xiao, Y.-Q. Zhang, Q.-L. 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).These compounds anchored covalently to various substrates by hydroxy-functioned represents one of the most interesting issues(Bella *et al.*, 2004). Here, the title compound (I) (1,3-bis(2-aminophenoxy)-2-propanol) was prepared from *o*-nitrophenol and epichlorohydrin , by etherization and reduction of nitro group.

In the crystal structure of the title compound (I), the two phenyl rings were linked by ethereal chain forming a non-coplanar structure (Fig. 1). Layers are formed by the intermolecular hydrogen bonds, and the aryl rings in different molecules are approximately parallel to each other. The O2 atom of the hydroxy group in (I) form two intermolecular hydrogen bonds with the N1 and N2 atoms of two adjeacent molecules, respectively (Fig. 2). The O2 atom is doubly hydrogen bridged. The N2···O2···N1 angle is about 112°. Thus, the molecular packing is controlled by hydrogen bonding interactions.

Experimental

80% Hydrazine hydrate (4.5 g, 72 mmol, 2.0 equiv.) was added slowly , whilst stirring, to a ethanol solution containing 1,3-bis(2-nitrophenoxy)-2-propanol (3.0 g, 9 mmol), $FeCl_3.6H_2O$ (0.8 g) and active carbon (1.8 g). The mixture was heated, and stirring for about 2 h. The black residue was removed from the solution by filtration, and then the solvent was removed under reduced pressure. The crude product was purified by column chromatography over silica gel using 20% EtOAc-hexane to afford pure yellow crystals, 1.7 g, in a yield of 69%. Single crystals of (I) suitable for X-ray diffraction were obtained from an ethanol-CH_2Cl_2 mixture by slow evaporation at room temperature.

Refinement

The H atoms in hydroxy group were located in a difference Fourier map and refine in their as-found positions relative to O atoms with U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were placed in calculated positions with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and refined using a riding model. U_{iso}(H) = 1.2-1.5U_{eq}(C,*N*).

Figures

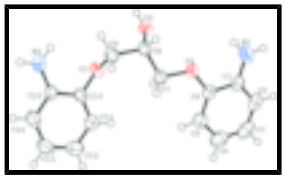

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

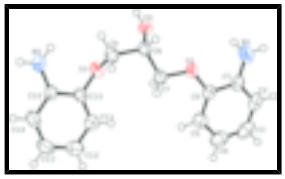

Fig. 2. packing diagram of (I). Hydrogen bonds are shown as dashed lines.

1,3-Bis(2-aminophenoxy)-2-propanol

Crystal data

$C_{15}H_{18}N_2O_3$	F_{000} = 584
M_r = 274.31	D_x = 1.327 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2382 reflections
a = 14.069 (2) Å	θ = 1.5–25.0º
b = 5.8636 (9) Å	μ = 0.09 mm^{-1}
c = 17.112 (3) Å	T = 293 (2) K
β = 103.418 (7)º	Prism, yellow
V = 1373.2 (4) Å^3	0.21 × 0.17 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2382 independent reflections
Radiation source: fine-focus sealed tube	1780 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −16→15
T_{min} = 0.981, T_{max} = 0.987	k = −6→5
9223 measured reflections	l = −20→20

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.31P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.146	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
S = 1.10	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
2382 reflections	Extinction correction: none
178 parameters	
Primary atom site location: structure-invariant direct methods	

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.81149 (16)	−0.0370 (4)	1.01642 (11)	0.0407 (5)
C2	0.74359 (18)	−0.1889 (4)	1.03225 (13)	0.0521 (6)
H2	0.7647	−0.3147	1.0648	0.063*
C3	0.64443 (19)	−0.1577 (5)	1.00061 (14)	0.0597 (7)
H3	0.5997	−0.2624	1.0117	0.072*
C4	0.61236 (18)	0.0277 (5)	0.95297 (15)	0.0618 (7)
H4	0.5458	0.0506	0.9328	0.074*
C5	0.67907 (16)	0.1809 (4)	0.93479 (13)	0.0518 (6)
H5	0.6573	0.3060	0.9021	0.062*
C6	0.77767 (14)	0.1480 (4)	0.96517 (11)	0.0385 (5)
C7	0.82321 (10)	0.4514 (2)	0.88735 (8)	0.0396 (5)
H7A	0.7834	0.5690	0.9037	0.048*
H7B	0.7856	0.3803	0.8388	0.048*
C8	0.91478 (10)	0.5536 (2)	0.87210 (8)	0.0372 (5)
H8	0.9573	0.5919	0.9244	0.045*
C9	0.89298 (15)	0.7733 (3)	0.82454 (12)	0.0405 (5)
H9A	0.8643	0.8836	0.8545	0.049*
H9B	0.9530	0.8371	0.8153	0.049*
C10	0.74699 (14)	0.8723 (3)	0.72770 (11)	0.0354 (5)
C11	0.65635 (15)	0.7980 (4)	0.73339 (13)	0.0492 (6)
H11	0.6497	0.6563	0.7560	0.059*
C12	0.57499 (18)	0.9325 (5)	0.70570 (15)	0.0610 (7)
H12	0.5135	0.8825	0.7096	0.073*
C13	0.58582 (18)	1.1407 (5)	0.67236 (14)	0.0604 (7)
H13	0.5312	1.2317	0.6532	0.072*
C14	0.67606 (17)	1.2160 (4)	0.66696 (13)	0.0512 (6)
H14	0.6819	1.3580	0.6443	0.061*
C15	0.75904 (14)	1.0847 (3)	0.69467 (10)	0.0364 (5)
N1	0.91044 (15)	−0.0606 (4)	1.04645 (13)	0.0733 (7)
H1A	0.9328	−0.1746	1.0768	0.088*

H1B	0.9500	0.0387	1.0349	0.088*
N2	0.85195 (13)	1.1623 (3)	0.69122 (10)	0.0459 (5)
H2A	0.8587	1.2946	0.6715	0.055*
H2B	0.9023	1.0777	0.7088	0.055*
O1	0.85053 (10)	0.2843 (2)	0.94980 (8)	0.0464 (4)
O2	0.96575 (9)	0.3940 (2)	0.83438 (8)	0.0430 (4)
H2C	1.0155	0.4535	0.8266	0.064*
O3	0.82630 (10)	0.7260 (2)	0.74908 (7)	0.0414 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0495 (13)	0.0407 (13)	0.0340 (10)	−0.0012 (10)	0.0137 (9)	0.0010 (9)
C2	0.0749 (17)	0.0417 (14)	0.0452 (12)	−0.0087 (12)	0.0248 (12)	0.0035 (10)
C3	0.0668 (17)	0.0579 (17)	0.0619 (14)	−0.0267 (14)	0.0298 (13)	−0.0086 (13)
C4	0.0450 (14)	0.0731 (19)	0.0681 (15)	−0.0120 (13)	0.0150 (12)	−0.0047 (14)
C5	0.0443 (13)	0.0573 (15)	0.0519 (12)	−0.0022 (12)	0.0075 (10)	0.0082 (12)
C6	0.0424 (12)	0.0379 (12)	0.0360 (10)	−0.0050 (10)	0.0108 (9)	0.0008 (9)
C7	0.0431 (12)	0.0365 (12)	0.0385 (10)	0.0043 (10)	0.0079 (9)	0.0070 (9)
C8	0.0389 (11)	0.0347 (12)	0.0382 (10)	0.0043 (9)	0.0092 (9)	0.0035 (9)
C9	0.0442 (12)	0.0311 (11)	0.0438 (11)	−0.0009 (9)	0.0054 (9)	0.0027 (9)
C10	0.0387 (12)	0.0322 (12)	0.0347 (10)	0.0055 (9)	0.0075 (8)	0.0007 (9)
C11	0.0464 (14)	0.0485 (14)	0.0538 (12)	0.0002 (11)	0.0140 (10)	0.0070 (11)
C12	0.0404 (13)	0.0744 (19)	0.0682 (15)	0.0035 (13)	0.0123 (11)	0.0030 (14)
C13	0.0481 (15)	0.0671 (18)	0.0634 (15)	0.0233 (13)	0.0076 (12)	0.0076 (14)
C14	0.0601 (15)	0.0419 (14)	0.0504 (13)	0.0144 (12)	0.0104 (11)	0.0104 (10)
C15	0.0429 (12)	0.0341 (12)	0.0328 (9)	0.0045 (10)	0.0103 (8)	0.0014 (9)
N1	0.0546 (13)	0.0726 (16)	0.0848 (15)	0.0004 (11)	−0.0002 (11)	0.0421 (13)
N2	0.0504 (11)	0.0350 (11)	0.0530 (10)	0.0024 (9)	0.0136 (8)	0.0103 (8)
O1	0.0404 (8)	0.0469 (9)	0.0497 (8)	−0.0050 (7)	0.0062 (7)	0.0189 (7)
O2	0.0381 (8)	0.0388 (9)	0.0551 (8)	0.0061 (7)	0.0169 (6)	0.0065 (7)
O3	0.0465 (9)	0.0337 (8)	0.0413 (8)	0.0091 (7)	0.0049 (6)	0.0019 (6)

Geometric parameters (Å, °)

C1—N1	1.375 (3)	C9—H9A	0.9700
C1—C2	1.378 (3)	C9—H9B	0.9700
C1—C6	1.407 (3)	C10—C11	1.372 (3)
C2—C3	1.387 (3)	C10—O3	1.388 (2)
C2—H2	0.9300	C10—C15	1.394 (3)
C3—C4	1.371 (4)	C11—C12	1.380 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.386 (3)	C12—C13	1.371 (4)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.377 (3)	C13—C14	1.367 (3)
C5—H5	0.9300	C13—H13	0.9300
C6—O1	1.373 (2)	C14—C15	1.387 (3)
C7—O1	1.4350 (19)	C14—H14	0.9300
C7—C8	1.4978	C15—N2	1.398 (3)

C7—H7A	0.9700	N1—H1A	0.8600
C7—H7B	0.9700	N1—H1B	0.8600
C8—O2	1.422 (2)	N2—H2A	0.8600
C8—C9	1.516 (2)	N2—H2B	0.8600
C8—H8	0.9800	O2—H2C	0.8200
C9—O3	1.436 (2)		
N1—C1—C2	123.3 (2)	C8—C9—H9A	109.9
N1—C1—C6	118.52 (19)	O3—C9—H9B	109.9
C2—C1—C6	118.1 (2)	C8—C9—H9B	109.9
C1—C2—C3	121.2 (2)	H9A—C9—H9B	108.3
C1—C2—H2	119.4	C11—C10—O3	119.26 (19)
C3—C2—H2	119.4	C11—C10—C15	120.98 (19)
C4—C3—C2	120.0 (2)	O3—C10—C15	119.54 (17)
C4—C3—H3	120.0	C10—C11—C12	120.3 (2)
C2—C3—H3	120.0	C10—C11—H11	119.9
C3—C4—C5	120.1 (2)	C12—C11—H11	119.9
C3—C4—H4	120.0	C13—C12—C11	119.2 (2)
C5—C4—H4	120.0	C13—C12—H12	120.4
C6—C5—C4	120.0 (2)	C11—C12—H12	120.4
C6—C5—H5	120.0	C14—C13—C12	120.7 (2)
C4—C5—H5	120.0	C14—C13—H13	119.7
O1—C6—C5	125.27 (19)	C12—C13—H13	119.7
O1—C6—C1	114.13 (17)	C13—C14—C15	121.2 (2)
C5—C6—C1	120.6 (2)	C13—C14—H14	119.4
O1—C7—C8	108.08 (8)	C15—C14—H14	119.4
O1—C7—H7A	110.1	C14—C15—C10	117.6 (2)
C8—C7—H7A	110.1	C14—C15—N2	121.7 (2)
O1—C7—H7B	110.1	C10—C15—N2	120.70 (17)
C8—C7—H7B	110.1	C1—N1—H1A	120.0
H7A—C7—H7B	108.4	C1—N1—H1B	120.0
O2—C8—C7	111.14 (8)	H1A—N1—H1B	120.0
O2—C8—C9	112.07 (13)	C15—N2—H2A	120.0
C7—C8—C9	110.99 (10)	C15—N2—H2B	120.0
O2—C8—H8	107.5	H2A—N2—H2B	120.0
C7—C8—H8	107.5	C6—O1—C7	117.22 (13)
C9—C8—H8	107.5	C8—O2—H2C	109.5
O3—C9—C8	109.11 (15)	C10—O3—C9	115.81 (15)
O3—C9—H9A	109.9		
N1—C1—C2—C3	179.9 (2)	C15—C10—C11—C12	0.5 (3)
C6—C1—C2—C3	−1.8 (3)	C10—C11—C12—C13	0.1 (4)
C1—C2—C3—C4	−0.3 (4)	C11—C12—C13—C14	−0.5 (4)
C2—C3—C4—C5	1.6 (4)	C12—C13—C14—C15	0.2 (4)
C3—C4—C5—C6	−0.5 (4)	C13—C14—C15—C10	0.5 (3)
C4—C5—C6—O1	178.3 (2)	C13—C14—C15—N2	−178.43 (19)
C4—C5—C6—C1	−1.7 (3)	C11—C10—C15—C14	−0.8 (3)
N1—C1—C6—O1	1.2 (3)	O3—C10—C15—C14	173.84 (17)
C2—C1—C6—O1	−177.11 (17)	C11—C10—C15—N2	178.09 (18)
N1—C1—C6—C5	−178.8 (2)	O3—C10—C15—N2	−7.3 (3)

C2—C1—C6—C5	2.9 (3)	C5—C6—O1—C7	−10.7 (3)
O1—C7—C8—O2	70.28 (11)	C1—C6—O1—C7	169.24 (16)
O1—C7—C8—C9	−164.28 (16)	C8—C7—O1—C6	−171.17 (12)
O2—C8—C9—O3	65.35 (19)	C11—C10—O3—C9	−105.4 (2)
C7—C8—C9—O3	−59.57 (16)	C15—C10—O3—C9	79.9 (2)
O3—C10—C11—C12	−174.1 (2)	C8—C9—O3—C10	132.46 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.86	2.24	3.061 (2)	161
N1—H1B···N1^{i}	0.86	2.66	3.353 (4)	139
N2—H2B···O2^{ii}	0.86	2.41	3.125 (2)	142
O2—H2C···N2^{iii}	0.82	2.31	3.125 (2)	173

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+2, *y*+1/2, −*z*+3/2; (iii) −*x*+2, *y*−1/2, −*z*+3/2.

Fig. 1

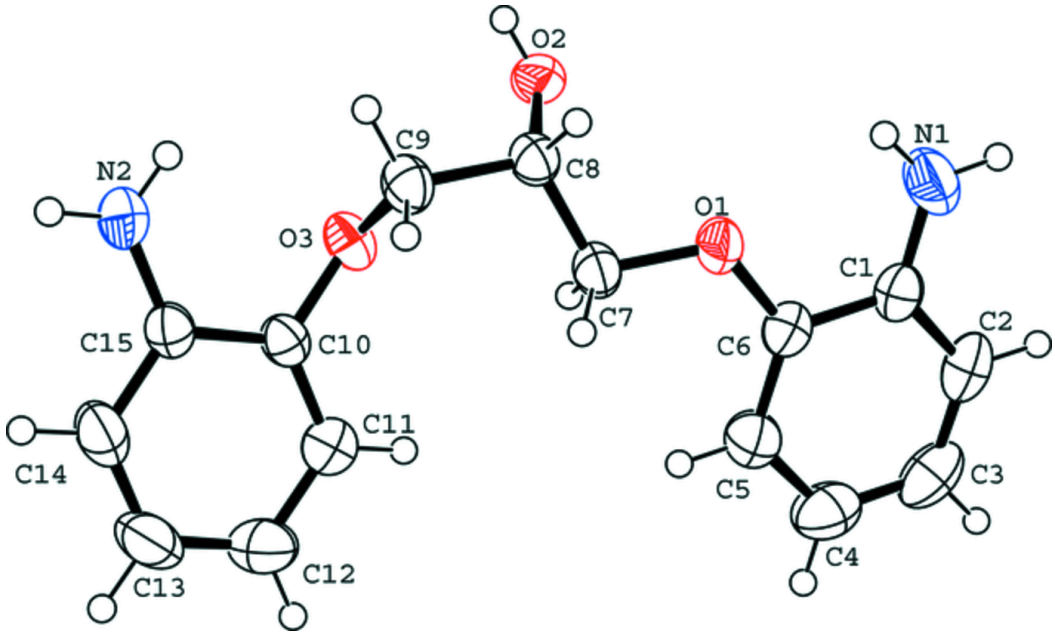

Fig. 2