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2,2′-Bis[4-(benzyloxy)phenyl]propane

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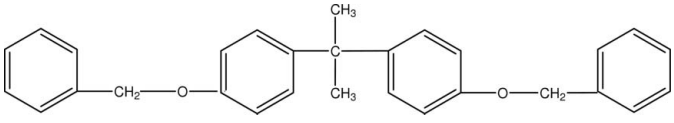
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.123; data-to-parameter ratio = 15.7.

The title compound, $C_{29}H_{28}O_2$, was obtained unintentionally as the product of an attempted synthesis of a new chiral cobalt salen catalyst [H_2salen is bis(salicylidene)ethylenediamine]. The asymmetric unit is one half-molecule; a crystallographic twofold rotation axis passes through the central C atom. In the crystal structure, intermolecular C—H$\cdots\pi$ interactions are found.

Related literature

For general background, see: Annis & Jacobsen (1999); Ready & Jacobsen (2001); Mi-ae & Geon (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{29}H_{28}O_2$
M_r = 408.51
Monoclinic, $C2/c$
a = 18.808 (4) Å
b = 6.3900 (13) Å
c = 18.925 (4) Å
β = 90.97 (3)°
V = 2274.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.966, T_{max} = 0.978
2918 measured reflections
2227 independent reflections
1558 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.05
2227 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$B\cdots Cg1^{i}$	0.97	2.78	3.488 (2)	131

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: HK2304).

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supplementary materials

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2,2'-Bis[4-(benzyloxy)phenyl]propane

G.-W. Wang, W.-Y. Wu and J.-T. Wang

Comment

Chiral Co(salen) complexes are widely used in the hydrolytic kinetic resolution of terminal epoxides, such as epichlorohydrin (Annis & Jacobsen, 1999). Bisphenols, such as bisphenol A, are useful as starting materials for the synthesis of salicylaldehyde (Ready & Jacobsen, 2001), especially in the synthesis of polymeric salen complexes (Mi-ae & Geon, 2003). The title compound, (I), was obtained unintentionally as the product of an attempted synthesis of a new chiral cobalt salen catalyst. We report herein the crystal structure of (I).

The asymmetric unit of the title compound, (I), contains one half molecule (Fig. 1), in which C14 atom lies on the twofold rotation axis. The bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

The rings A (C1—C6) and B (C8—C13) are, of course, planar and the dihedral angle between them is 76.5 (3)°.

In the crystal structure, intermolecular C—H···π interactions involving ring A (Table1), linking the molecules (Fig. 2, where cg1 is the centroid of ring A), seem to be effective in the stabilization of the structure.

Experimental

Under nitrogen atmosphere, a mixture of bisphenol A (7.5 g, 33 mmol) and anhydrous potassium carbonate (2.2 g, 16 mmol) in dry acetonitrile (75 ml) were stirred for half an hour at room temperature. Subsequently benzyl chloride (8.2 g, 66 mmol) and potassium iodide (0.6 g, 3.6 mmol) were added to the reaction mixture, which was then refluxed for another 3 h, in inert atmosphere. The mixture was cooled to room temperature, filtrated and the solvent was removed under reduced pressure. The crude product was purified with n-hexane solution. Crystals of (I) suitable for X-ray diffraction were recrystallized by slow evaporation of acetone.

Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Figures

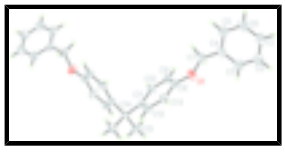

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

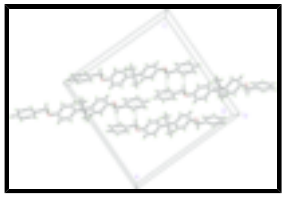

Fig. 2. A partial packing diagram of (I). C—H···π interactions are shown as dashed lines.

2,2'-Bis[4-(benzyloxy)phenyl]propane

Crystal data

$C_{29}H_{28}O_2$	F_{000} = 872
M_r = 408.51	D_x = 1.193 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 25 reflections
a = 18.808 (4) Å	θ = 9–13º
b = 6.3900 (13) Å	μ = 0.07 mm^{-1}
c = 18.925 (4) Å	*T* = 298 (2) K
β = 90.97 (3)º	Block, colorless
V = 2274.1 (8) Å^3	0.40 × 0.30 × 0.30 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.040
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 2.2º
T = 298(2) K	*h* = −22→22
ω/2θ scans	*k* = 0→7
Absorption correction: ψ scan (North *et al.*, 1968)	*l* = 0→23
T_{min} = 0.966, T_{max} = 0.978	3 standard reflections
2918 measured reflections	every 200 reflections
2227 independent reflections	intensity decay: none
1558 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.123	$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.7301P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2227 reflections	$\Delta\rho_{max}$ = 0.13 e Å^{-3}

142 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
O1	0.23856 (6)	0.1080 (2)	0.36046 (6)	0.0573 (4)
C1	0.43148 (10)	−0.2644 (4)	0.48738 (12)	0.0712 (6)
H1	0.4754	−0.3060	0.5057	0.085*
C2	0.40194 (11)	−0.0813 (4)	0.50883 (13)	0.0766 (6)
H2	0.4255	0.0019	0.5420	0.092*
C3	0.33710 (10)	−0.0191 (3)	0.48132 (12)	0.0694 (6)
H3	0.3173	0.1061	0.4964	0.083*
C4	0.30101 (9)	−0.1383 (3)	0.43194 (10)	0.0551 (5)
C5	0.33134 (11)	−0.3246 (3)	0.41111 (10)	0.0688 (6)
H5	0.3079	−0.4089	0.3781	0.083*
C6	0.39667 (11)	−0.3867 (4)	0.43914 (11)	0.0746 (6)
H6	0.4168	−0.5124	0.4249	0.090*
C7	0.22947 (9)	−0.0712 (3)	0.40375 (11)	0.0659 (6)
H7A	0.2080	−0.1836	0.3763	0.079*
H7B	0.1983	−0.0383	0.4426	0.079*
C8	0.17851 (8)	0.2026 (3)	0.33329 (8)	0.0446 (4)
C9	0.10960 (9)	0.1519 (3)	0.35085 (9)	0.0522 (5)
H9	0.1010	0.0431	0.3822	0.063*
C10	0.05346 (8)	0.2643 (3)	0.32147 (9)	0.0515 (4)
H10	0.0073	0.2276	0.3333	0.062*
C11	0.06324 (8)	0.4287 (2)	0.27526 (8)	0.0411 (4)
C12	0.13292 (9)	0.4733 (3)	0.25751 (9)	0.0530 (5)
H12	0.1416	0.5804	0.2255	0.064*
C13	0.18954 (9)	0.3632 (3)	0.28597 (9)	0.0559 (5)
H13	0.2356	0.3974	0.2732	0.067*
C14	0.0000	0.5628 (4)	0.2500	0.0472 (6)
C15	−0.02072 (10)	0.7045 (3)	0.31224 (11)	0.0697 (6)
H15A	−0.0571	0.8003	0.2970	0.105*
H15B	0.0202	0.7815	0.3284	0.105*
H15C	−0.0382	0.6197	0.3501	0.105*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0413 (6)	0.0677 (8)	0.0629 (7)	0.0058 (6)	−0.0017 (5)	0.0181 (7)
C1	0.0481 (11)	0.0874 (16)	0.0779 (14)	0.0098 (11)	−0.0046 (10)	0.0149 (13)
C2	0.0629 (13)	0.0765 (14)	0.0896 (15)	−0.0036 (12)	−0.0204 (11)	0.0023 (13)
C3	0.0600 (12)	0.0576 (12)	0.0903 (15)	0.0061 (10)	−0.0081 (11)	−0.0012 (11)
C4	0.0478 (10)	0.0609 (12)	0.0566 (11)	0.0027 (9)	−0.0028 (8)	0.0118 (9)
C5	0.0747 (13)	0.0755 (14)	0.0560 (11)	0.0100 (11)	−0.0072 (9)	−0.0065 (11)
C6	0.0708 (13)	0.0808 (15)	0.0725 (14)	0.0305 (12)	0.0074 (11)	0.0029 (12)
C7	0.0518 (11)	0.0687 (13)	0.0768 (13)	0.0020 (10)	−0.0090 (9)	0.0218 (11)
C8	0.0411 (9)	0.0500 (10)	0.0427 (8)	0.0034 (7)	−0.0041 (7)	−0.0008 (8)
C9	0.0466 (9)	0.0532 (10)	0.0566 (10)	−0.0050 (8)	−0.0052 (8)	0.0175 (9)
C10	0.0379 (8)	0.0553 (11)	0.0612 (11)	−0.0059 (8)	−0.0028 (7)	0.0130 (9)
C11	0.0424 (9)	0.0401 (9)	0.0408 (8)	−0.0042 (7)	−0.0041 (7)	−0.0019 (7)
C12	0.0503 (10)	0.0558 (11)	0.0529 (10)	−0.0034 (8)	0.0011 (8)	0.0163 (9)
C13	0.0400 (9)	0.0685 (12)	0.0594 (11)	−0.0025 (9)	0.0037 (8)	0.0149 (10)
C14	0.0469 (13)	0.0385 (12)	0.0558 (14)	0.000	−0.0077 (10)	0.000
C15	0.0620 (12)	0.0571 (12)	0.0894 (15)	0.0054 (10)	−0.0155 (10)	−0.0279 (11)

Geometric parameters (Å, °)

C1—C2	1.360 (3)	C8—C9	1.382 (2)
C1—C6	1.361 (3)	C9—C10	1.386 (2)
C1—H1	0.9300	C9—H9	0.9300
C2—C3	1.376 (3)	C10—C11	1.381 (2)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.376 (3)	C11—C12	1.388 (2)
C3—H3	0.9300	C11—C14	1.536 (2)
C4—C5	1.381 (3)	C12—C13	1.378 (2)
C4—C7	1.501 (2)	C12—H12	0.9300
C5—C6	1.388 (3)	C13—H13	0.9300
C5—H5	0.9300	C14—C11^{i}	1.536 (2)
C6—H6	0.9300	C14—C15^{i}	1.541 (2)
C7—O1	1.420 (2)	C14—C15	1.541 (2)
C7—H7A	0.9700	C15—H15A	0.9600
C7—H7B	0.9700	C15—H15B	0.9600
C8—O1	1.3731 (18)	C15—H15C	0.9600
C8—C13	1.380 (2)		
C2—C1—C6	119.99 (19)	C8—C9—H9	120.2
C2—C1—H1	120.0	C10—C9—H9	120.2
C6—C1—H1	120.0	C11—C10—C9	122.65 (15)
C1—C2—C3	119.9 (2)	C11—C10—H10	118.7
C1—C2—H2	120.0	C9—C10—H10	118.7
C3—C2—H2	120.0	C10—C11—C12	116.49 (15)
C4—C3—C2	121.4 (2)	C10—C11—C14	120.71 (13)
C4—C3—H3	119.3	C12—C11—C14	122.65 (14)

C2—C3—H3	119.3	C13—C12—C11	121.80 (16)
C3—C4—C5	118.03 (17)	C13—C12—H12	119.1
C3—C4—C7	120.83 (18)	C11—C12—H12	119.1
C5—C4—C7	121.10 (18)	C12—C13—C8	120.63 (15)
C4—C5—C6	120.31 (19)	C12—C13—H13	119.7
C4—C5—H5	119.8	C8—C13—H13	119.7
C6—C5—H5	119.8	C11^{i}—C14—C11	112.16 (18)
C1—C6—C5	120.3 (2)	C11^{i}—C14—C15^{i}	107.12 (9)
C1—C6—H6	119.8	C11—C14—C15^{i}	111.17 (9)
C5—C6—H6	119.8	C11^{i}—C14—C15	111.17 (9)
O1—C7—C4	108.61 (15)	C11—C14—C15	107.12 (9)
O1—C7—H7A	110.0	C15^{i}—C14—C15	108.1 (2)
C4—C7—H7A	110.0	C14—C15—H15A	109.5
O1—C7—H7B	110.0	C14—C15—H15B	109.5
C4—C7—H7B	110.0	H15A—C15—H15B	109.5
H7A—C7—H7B	108.3	C14—C15—H15C	109.5
O1—C8—C13	116.00 (14)	H15A—C15—H15C	109.5
O1—C8—C9	125.14 (15)	H15B—C15—H15C	109.5
C13—C8—C9	118.84 (15)	C8—O1—C7	117.69 (13)
C8—C9—C10	119.56 (16)		
C6—C1—C2—C3	−0.5 (3)	C10—C11—C12—C13	−1.7 (3)
C1—C2—C3—C4	−0.2 (3)	C14—C11—C12—C13	173.81 (15)
C2—C3—C4—C5	0.8 (3)	C11—C12—C13—C8	0.3 (3)
C2—C3—C4—C7	178.4 (2)	O1—C8—C13—C12	−177.72 (16)
C3—C4—C5—C6	−0.6 (3)	C9—C8—C13—C12	1.0 (3)
C7—C4—C5—C6	−178.30 (19)	C10—C11—C14—C11^{i}	−48.19 (12)
C2—C1—C6—C5	0.6 (3)	C12—C11—C14—C11^{i}	136.45 (17)
C4—C5—C6—C1	0.0 (3)	C10—C11—C14—C15^{i}	−168.10 (15)
C3—C4—C7—O1	69.8 (2)	C12—C11—C14—C15^{i}	16.5 (2)
C5—C4—C7—O1	−112.6 (2)	C10—C11—C14—C15	74.1 (2)
O1—C8—C9—C10	177.77 (16)	C12—C11—C14—C15	−101.31 (17)
C13—C8—C9—C10	−0.8 (3)	C13—C8—O1—C7	−173.80 (16)
C8—C9—C10—C11	−0.7 (3)	C9—C8—O1—C7	7.6 (3)
C9—C10—C11—C12	1.9 (3)	C4—C7—O1—C8	−175.67 (15)
C9—C10—C11—C14	−173.71 (16)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7B···Cg1^{ii}	0.97	2.78	3.488 (2)	131

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

Fig. 1

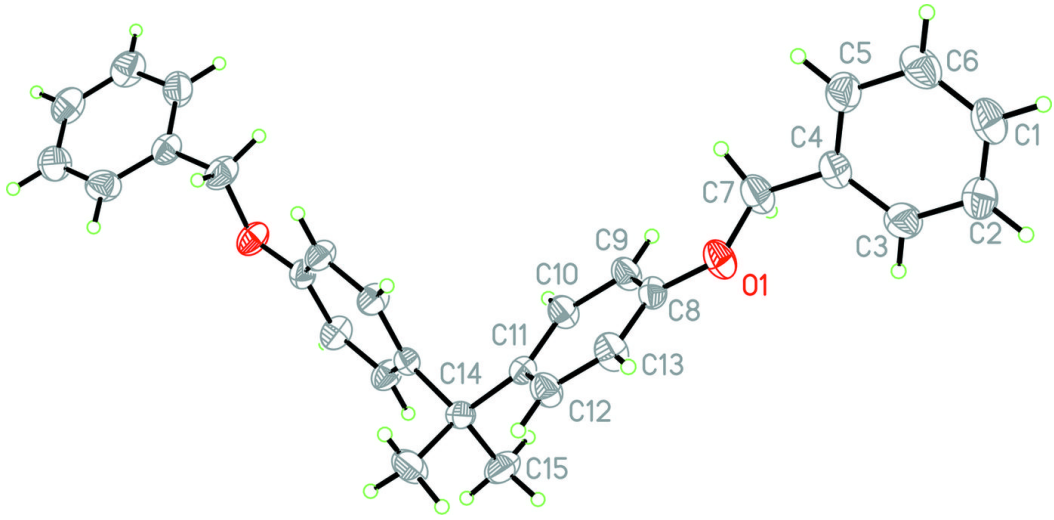

Fig. 2