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1-[(2-Hydroxy-1-naphthyl)(phenyl)methyl]-2-naphthol ethanol solvate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.051
wR factor = 0.139
Data-to-parameter ratio = 17.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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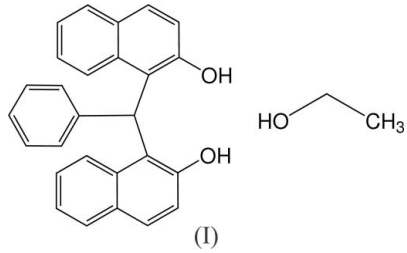
In the title compound, $C_{27}H_{20}O_2\cdot C_2H_6O$, intra- and intermolecular O—H···O hydrogen bonds link the molecules and seem to be effective in the stabilization of the crystal structure. All the H atoms in the hydroxyl groups are disordered.

Comment

Bisnaphthols are usually referred to as a diverse group of synthetic compounds containing two naphthol units which are connected by an aldehyde group. They have synthetic, medicinal and industrial value. They are structural units of calixarenes, and have applications as enzyme mimetics, ion-selective electrodes or sensors, selective membranes, non-linear optical materials and sometimes, with some modifications, as high-performance liquid chromatography stationary phases (Vries & Lefort, 2006; Handique & Barauh, 2002). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation. We report here the synthesis and crystal structure of (I).



(I)

The asymmetric unit of (I) contains an ethanol solvent molecule (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

Rings *A* (C1–C6), *B* (C1/C6–C10), *C* (C12–C16/C21), *D* (C16–C21) and *E* (C22–C27) are, of course, planar. The dihedral angles between rings *A* and *B*, and between rings *C* and *D*, are 3.34 (4) and 0.45 (3)°, respectively. The orientation of ring *E* with respect to the mean planes of the two naphthyl groups containing rings *A* and *B*, and *C* and *D*, may be described by the dihedral angles of 88.39 (3) and 64.62 (4)°, respectively. The dihedral angle between the mean planes of the two naphthyl groups is 73.79 (4)°.

The H atoms for all hydroxyl groups are disordered. First, we treated only the ethanol H atoms as disordered, and then extended that to the whole O—H···O network.

As can be seen from the packing diagram (Fig. 2), intra- and intermolecular O—H···O hydrogen bonds (Table 1) link the molecules, and may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

Concentrated hydrochloric acid (0.2 ml) was added to 2-naphthol (1.00 g, 7.0 mmol) and benzaldehyde (0.37 g, 3.5 mmol) in acetic acid (5 ml) at 273 K and the mixture was kept for 50 h in a refrigerator. The pink–white precipitate was filtered off and washed copiously with water. Crystals of (I) suitable for X-ray analysis were obtained by recrystallization from ethanol (yield 1.7 g, 64%; m.p. 462–463 K).

Crystal data

$C_{27}H_{20}O_2\cdot C_2H_6O$
$M_r = 422.5$
Triclinic, $P\overline{1}$
$a = 8.691$ (2) Å
$b = 10.8185$ (13) Å
$c = 12.492$ (4) Å
$\alpha = 82.20$ (2)°
$\beta = 78.20$ (2)°
$\gamma = 73.872$ (15)°
$V = 1100.6$ (5) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298$ K
0.43 × 0.41 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: none
22213 measured reflections
5033 independent reflections
3736 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.139$
$S = 1.02$
5033 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1OA···O2	0.90	1.75	2.6080 (19)	158
O1—H1OB···O1^{i}	0.94	1.84	2.7713 (17)	170
O2O—H2A···O3	0.87	1.78	2.646 (2)	172
O3—H3B···O3^{ii}	0.85	1.83	2.6817 (19)	180

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

H atoms were located in difference density maps and treated as riding on the respective carrier atom, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(parent atom). H atoms involved in hydrogen bonds were refined using a disordered model with 50% occupancy for both positions.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *maXus* (Mackay *et al.*, 1999).

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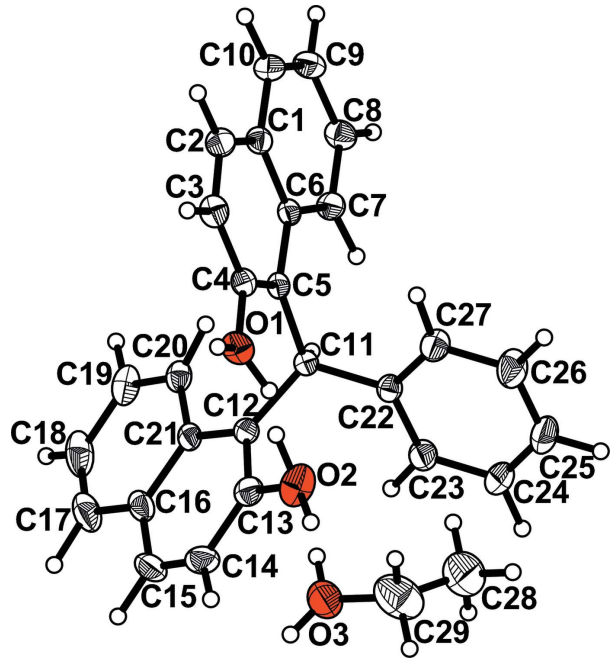

Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Both disorder components are shown for each OH group.

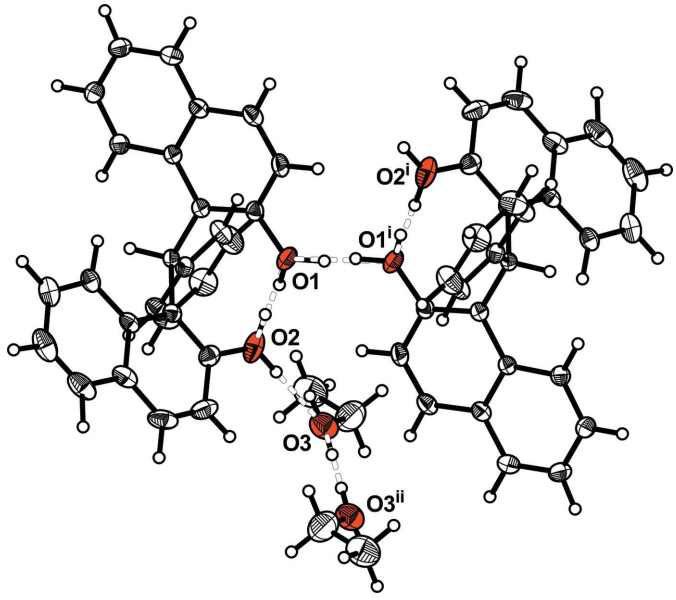

Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines. Both disorder components are shown for each OH group. [Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $1-x, -1-y, 1-z$.]

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