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3-(*p*-Tolyliminomethyl)-1,1′-binaphthol ethanol solvate

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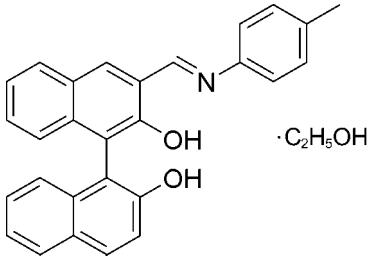
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.188; data-to-parameter ratio = 13.8.

The binaphthol backbone in the title compound, $C_{28}H_{21}NO_2\cdot C_2H_5OH$, suggests that it has potential for use in asymmetric synthesis with both hydroxy groups and the imino group providing sites for coordination with metal ions as an O/N heterotridentate ligand. There is one intramolecular O—H···N hydrogen bond that forms a five-membered ring and two intermolecular O—H···O hydrogen bonds to the ethanol solvent, linking two ethanol molecules and two naphthol molecules around a center of symmetry.

Related literature

For background on the application of salen complexes to asymmetric catalysis see: Raffaelli *et al.* (1998); for synthesis see Chin *et al.* (2004).



Experimental

Crystal data

$C_{28}H_{21}NO_2\cdot C_2H_6O$
M_r = 449.53
Triclinic, $P\overline{1}$
a = 10.540 (5) Å
b = 10.740 (3) Å
c = 10.779 (3) Å
α = 82.17 (2)°
β = 83.82 (3)°
γ = 82.89 (3)°
V = 1194.4 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 292 (2) K
0.26 × 0.25 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
4426 measured reflections
4391 independent reflections
2054 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
3 standard reflections
every 300 reflections
intensity decay: 3.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.188
S = 0.94
4391 reflections
319 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3	0.82	1.95	2.753 (3)	164
O2—H2···N	0.80 (4)	1.90 (4)	2.612 (3)	148 (4)
O3—H3A···O2^{i}	0.82	2.08	2.844 (3)	155

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); 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) and *Mercury* (Version 1.2; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2134).

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supplementary materials

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3-(*p*-Tolyliminomethyl)-1,1'-binaphthol ethanol solvate

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Comment

Copper and manganese complexes containing Schiff bases as ligands have potential interest in homogeneous catalysis(Raffaelli *et al.*, 1998)·In this paper, we present and X-ray crystallographic analysis of the title compound (I), as a continuation of our previous studies. The binol backbone indicates that it has potential as a ligand in asymmetric synthesis.

As shown in Fig. 1, an intramolecular O—H···N hydrogen bond forms a five–membered ring. Both hydroxyl group and the imino moiety provide potential sites for coordination with metal ions as a O/N heterotridenate ligand.

The compounds (I) are connected by O—H···O hydrogen bonds to the ethanol, Fig 2.

In the crystal structure there are close approaches between the ring systems in neighboring molecules, for example, C11–15, 20 and C11–15, 20 rings, C11–15, 20 and C15–20 rings, and C11–15, 20 and C22–27 rings, the corresponding distances between ring centroids are 3.875 Å, 3.956Å and 4.110 Å.

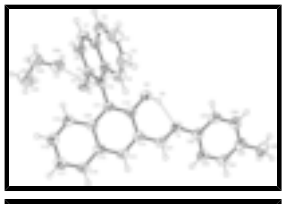
Experimental

The salen ligand, 3-((*p*-tolylimino)methyl)-di-1,1'-binaphthol was prepared by condensation of 3-carboxaldehyde-1,1'-binaphthol with *p*-toluidine, which was prepared in reported methods (Chin, J. *et al.*, 2004)·Crystals suitable for X-ray analysis were obtained by slow evaporation of a ethanol /methylene chloride (1:5) solution of the compound.

Refinement

H2 was located in a difference Fourier map and refined with restraints on the O—H distance. The remaining H atoms were placed in calculated positions and refined in the riding-model approximation.

Figures



Scheme 1

Fig. 1. A perspective view, with displacement ellipsoids drawn at the 30% propability level.

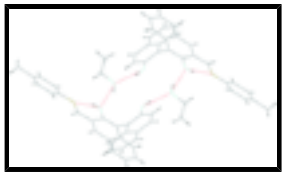


Fig. 2. Intermolecular hydrogen bonding in the crystal structure of (I).

3-(*p*-Tolyliminomethyl)-1,1'-binaphthol ethanol solvate

Crystal data

$C_{28}H_{21}NO_2 \cdot C_2H_6O$	$Z = 2$
$M_r = 449.53$	$F_{000} = 476$
Triclinic, $P\overline{1}$	$D_x = 1.250$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.540$ (5) Å	Cell parameters from 24 reflections
$b = 10.740$ (3) Å	$\theta = 4.8$–9.1º
$c = 10.779$ (3) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 82.17$ (2)º	$T = 292$ (2) K
$\beta = 83.82$ (3)º	Block, orange
$\gamma = 82.89$ (3)º	0.26 × 0.25 × 0.13 mm
$V = 1194.4$ (8) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.010$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.5$º
Monochromator: graphite	$\theta_{min} = 1.9$º
$T = 294(2)$ K	$h = -12 \rightarrow 12$
$\omega/2\theta$ scans	$k = -4 \rightarrow 12$
Absorption correction: none	$l = -12 \rightarrow 13$
4426 measured reflections	3 standard reflections
4391 independent reflections	every 300 reflections
2054 reflections with $I > 2\sigma(I)$	intensity decay: 3.2%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.188$	$w = 1/[\s^2^(F_o^2^) + (0.1107P)^2^]$ where $P = (F_o^2^ + 2F_c^2^)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} < 0.001$
4391 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
319 parameters	$\Delta\rho_{min} = -0.24$ 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	0.0738 (2)	0.3272 (2)	0.5630 (2)	0.0734 (7)
H1	0.0534	0.3780	0.6139	0.110 (11)*
O2	0.0508 (2)	0.27804 (19)	0.2159 (2)	0.0599 (6)
H2	0.007 (4)	0.264 (4)	0.164 (4)	0.100 (15)*
N	−0.0886 (2)	0.1489 (2)	0.1058 (2)	0.0507 (6)
C1	0.3334 (3)	0.3271 (2)	0.3103 (3)	0.0466 (7)
C2	0.3843 (3)	0.2626 (3)	0.2077 (3)	0.0569 (8)
H2A	0.3479	0.1920	0.1929	0.073 (2)*
C3	0.4861 (3)	0.3018 (3)	0.1295 (3)	0.0709 (10)
H3	0.5179	0.2577	0.0622	0.073 (2)*
C4	0.5433 (3)	0.4069 (3)	0.1490 (3)	0.0729 (10)
H4	0.6120	0.4330	0.0942	0.073 (2)*
C5	0.4991 (3)	0.4711 (3)	0.2475 (3)	0.0623 (8)
H5	0.5387	0.5404	0.2605	0.073 (2)*
C6	0.3942 (3)	0.4345 (2)	0.3307 (3)	0.0489 (7)
C7	0.3423 (3)	0.5013 (3)	0.4312 (3)	0.0567 (8)
H7	0.3812	0.5701	0.4465	0.073 (2)*
C8	0.2379 (3)	0.4687 (3)	0.5060 (3)	0.0611 (8)
H8	0.2045	0.5163	0.5703	0.073 (2)*
C9	0.1779 (3)	0.3613 (2)	0.4873 (3)	0.0510 (7)
C10	0.2273 (3)	0.2907 (2)	0.3919 (3)	0.0454 (7)
C11	0.1714 (3)	0.1708 (2)	0.3783 (2)	0.0451 (7)
C12	0.0883 (3)	0.1695 (2)	0.2894 (3)	0.0455 (7)
C13	0.0378 (3)	0.0548 (2)	0.2726 (2)	0.0445 (7)
C14	0.0729 (3)	−0.0547 (2)	0.3489 (2)	0.0450 (7)
H14	0.0388	−0.1284	0.3400	0.073 (2)*
C15	0.1591 (3)	−0.0574 (2)	0.4397 (2)	0.0440 (7)
C16	0.1966 (3)	−0.1712 (3)	0.5162 (3)	0.0526 (8)
H16	0.1611	−0.2444	0.5081	0.073 (2)*
C17	0.2839 (3)	−0.1750 (3)	0.6016 (3)	0.0620 (8)
H17	0.3086	−0.2501	0.6513	0.073 (2)*
C18	0.3356 (3)	−0.0639 (3)	0.6129 (3)	0.0657 (9)
H18	0.3965	−0.0669	0.6700	0.073 (2)*

C19	0.3007 (3)	0.0483 (3)	0.5442 (3)	0.0567 (8)
H19	0.3362	0.1204	0.5562	0.073 (2)*
C20	0.2104 (3)	0.0561 (2)	0.4543 (2)	0.0444 (7)
C21	−0.0490 (3)	0.0512 (3)	0.1792 (3)	0.0484 (7)
H21	−0.0776	−0.0258	0.1718	0.073 (2)*
C22	−0.1786 (3)	0.1411 (3)	0.0189 (3)	0.0482 (7)
C23	−0.2544 (3)	0.0420 (3)	0.0260 (3)	0.0579 (8)
H23	−0.2474	−0.0246	0.0906	0.073 (2)*
C24	−0.3389 (3)	0.0430 (3)	−0.0618 (3)	0.0568 (8)
H24	−0.3867	−0.0250	−0.0572	0.073 (2)*
C25	−0.3554 (3)	0.1417 (3)	−0.1573 (3)	0.0567 (8)
C26	−0.2799 (3)	0.2399 (3)	−0.1640 (3)	0.0606 (8)
H26	−0.2877	0.3069	−0.2282	0.073 (2)*
C27	−0.1936 (3)	0.2392 (3)	−0.0768 (3)	0.0561 (8)
H27	−0.1443	0.3062	−0.0827	0.073 (2)*
C28	−0.4529 (3)	0.1425 (3)	−0.2510 (3)	0.0725 (10)
H28A	−0.5307	0.1145	−0.2076	0.172 (9)*
H28B	−0.4191	0.0868	−0.3120	0.172 (9)*
H28C	−0.4708	0.2268	−0.2927	0.172 (9)*
O3	0.0233 (2)	0.4606 (2)	0.7668 (2)	0.0754 (7)
H3A	−0.0169	0.5313	0.7612	0.110 (11)*
C29	0.1223 (4)	0.4550 (4)	0.8508 (4)	0.0950 (13)
H29A	0.0844	0.4794	0.9312	0.170 (16)*
H29B	0.1837	0.5136	0.8158	0.170 (16)*
C30	0.1883 (5)	0.3249 (5)	0.8689 (5)	0.1227 (17)
H30A	0.2597	0.3233	0.9177	0.172 (9)*
H30B	0.2188	0.2983	0.7885	0.172 (9)*
H30C	0.1294	0.2688	0.9124	0.172 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0815 (17)	0.0628 (14)	0.0813 (16)	−0.0284 (12)	0.0206 (13)	−0.0314 (12)
O2	0.0766 (16)	0.0398 (11)	0.0687 (14)	−0.0135 (10)	−0.0299 (12)	−0.0018 (10)
N	0.0520 (15)	0.0505 (14)	0.0535 (14)	−0.0095 (11)	−0.0157 (12)	−0.0093 (12)
C1	0.0484 (17)	0.0425 (15)	0.0506 (16)	−0.0025 (13)	−0.0132 (14)	−0.0073 (13)
C2	0.059 (2)	0.0532 (17)	0.0617 (19)	−0.0109 (15)	−0.0057 (16)	−0.0137 (15)
C3	0.067 (2)	0.076 (2)	0.070 (2)	−0.0011 (18)	0.0040 (19)	−0.0255 (18)
C4	0.062 (2)	0.073 (2)	0.082 (2)	−0.0127 (18)	0.0097 (18)	−0.009 (2)
C5	0.064 (2)	0.0551 (19)	0.071 (2)	−0.0166 (16)	−0.0079 (18)	−0.0086 (16)
C6	0.0522 (18)	0.0390 (15)	0.0577 (17)	−0.0076 (13)	−0.0130 (14)	−0.0054 (13)
C7	0.066 (2)	0.0492 (17)	0.0615 (19)	−0.0230 (15)	−0.0092 (17)	−0.0112 (14)
C8	0.078 (2)	0.0469 (17)	0.0623 (19)	−0.0144 (16)	−0.0024 (17)	−0.0166 (15)
C9	0.0591 (19)	0.0429 (15)	0.0546 (17)	−0.0144 (14)	−0.0032 (15)	−0.0123 (14)
C10	0.0442 (17)	0.0424 (15)	0.0528 (17)	−0.0098 (12)	−0.0124 (14)	−0.0063 (13)
C11	0.0482 (17)	0.0383 (15)	0.0526 (16)	−0.0085 (12)	−0.0079 (14)	−0.0135 (13)
C12	0.0491 (17)	0.0358 (15)	0.0532 (17)	−0.0065 (12)	−0.0074 (14)	−0.0073 (13)
C13	0.0442 (16)	0.0420 (15)	0.0508 (16)	−0.0078 (12)	−0.0064 (13)	−0.0141 (13)

C14	0.0471 (17)	0.0368 (15)	0.0542 (17)	−0.0097 (12)	−0.0012 (14)	−0.0150 (13)
C15	0.0437 (17)	0.0387 (15)	0.0497 (16)	−0.0033 (12)	−0.0015 (13)	−0.0090 (12)
C16	0.060 (2)	0.0384 (15)	0.0595 (18)	−0.0057 (13)	−0.0017 (16)	−0.0076 (13)
C17	0.070 (2)	0.0507 (18)	0.062 (2)	0.0003 (15)	−0.0131 (17)	0.0014 (15)
C18	0.070 (2)	0.064 (2)	0.067 (2)	−0.0052 (17)	−0.0264 (17)	−0.0092 (17)
C19	0.061 (2)	0.0501 (17)	0.0634 (19)	−0.0105 (14)	−0.0183 (16)	−0.0095 (15)
C20	0.0441 (17)	0.0435 (15)	0.0482 (16)	−0.0068 (12)	−0.0064 (13)	−0.0117 (12)
C21	0.0450 (17)	0.0456 (16)	0.0598 (18)	−0.0108 (13)	−0.0067 (14)	−0.0182 (14)
C22	0.0436 (17)	0.0497 (16)	0.0535 (17)	−0.0061 (13)	−0.0048 (14)	−0.0132 (14)
C23	0.058 (2)	0.0542 (18)	0.0637 (19)	−0.0142 (15)	−0.0085 (16)	−0.0064 (15)
C24	0.0517 (19)	0.0571 (18)	0.069 (2)	−0.0146 (14)	−0.0073 (16)	−0.0231 (16)
C25	0.0490 (19)	0.068 (2)	0.0565 (18)	−0.0022 (15)	−0.0049 (15)	−0.0234 (16)
C26	0.060 (2)	0.064 (2)	0.0589 (19)	−0.0088 (16)	−0.0124 (16)	−0.0061 (16)
C27	0.056 (2)	0.0501 (17)	0.0644 (19)	−0.0127 (14)	−0.0061 (16)	−0.0082 (15)
C28	0.055 (2)	0.097 (3)	0.075 (2)	−0.0125 (18)	−0.0226 (18)	−0.025 (2)
O3	0.0790 (18)	0.0612 (15)	0.0881 (17)	−0.0015 (12)	−0.0025 (14)	−0.0261 (13)
C29	0.095 (3)	0.099 (3)	0.097 (3)	−0.006 (3)	−0.022 (3)	−0.025 (2)
C30	0.108 (4)	0.110 (4)	0.139 (4)	0.014 (3)	−0.016 (3)	0.005 (3)

Geometric parameters (Å, °)

O1—C9	1.352 (3)	C15—C20	1.427 (3)
O1—H1	0.8200	C16—C17	1.364 (4)
O2—C12	1.358 (3)	C16—H16	0.9300
O2—H2	0.80 (4)	C17—C18	1.397 (4)
N—C21	1.280 (3)	C17—H17	0.9300
N—C22	1.420 (4)	C18—C19	1.357 (4)
C1—C2	1.407 (4)	C18—H18	0.9300
C1—C10	1.408 (4)	C19—C20	1.417 (4)
C1—C6	1.439 (4)	C19—H19	0.9300
C2—C3	1.363 (4)	C21—H21	0.9300
C2—H2A	0.9300	C22—C27	1.377 (4)
C3—C4	1.394 (5)	C22—C23	1.397 (4)
C3—H3	0.9300	C23—C24	1.366 (4)
C4—C5	1.354 (4)	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.382 (4)
C5—C6	1.407 (4)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.387 (4)
C6—C7	1.405 (4)	C25—C28	1.515 (4)
C7—C8	1.346 (4)	C26—C27	1.375 (4)
C7—H7	0.9300	C26—H26	0.9300
C8—C9	1.429 (4)	C27—H27	0.9300
C8—H8	0.9300	C28—H28A	0.9600
C9—C10	1.379 (4)	C28—H28B	0.9600
C10—C11	1.512 (3)	C28—H28C	0.9600
C11—C12	1.368 (4)	O3—C29	1.444 (4)
C11—C20	1.425 (4)	O3—H3A	0.8200
C12—C13	1.441 (3)	C29—C30	1.480 (6)
C13—C14	1.375 (4)	C29—H29A	0.9700

C13—C21	1.439 (4)	C29—H29B	0.9700
C14—C15	1.400 (4)	C30—H30A	0.9600
C14—H14	0.9300	C30—H30B	0.9600
C15—C16	1.417 (4)	C30—H30C	0.9600
C9—O1—H1	109.5	C16—C17—H17	120.7
C12—O2—H2	111 (3)	C18—C17—H17	120.7
C21—N—C22	120.8 (2)	C19—C18—C17	122.7 (3)
C2—C1—C10	122.8 (3)	C19—C18—H18	118.6
C2—C1—C6	117.5 (3)	C17—C18—H18	118.6
C10—C1—C6	119.7 (2)	C18—C19—C20	120.3 (3)
C3—C2—C1	121.1 (3)	C18—C19—H19	119.9
C3—C2—H2A	119.4	C20—C19—H19	119.9
C1—C2—H2A	119.4	C19—C20—C11	122.8 (2)
C2—C3—C4	121.0 (3)	C19—C20—C15	117.6 (3)
C2—C3—H3	119.5	C11—C20—C15	119.6 (2)
C4—C3—H3	119.5	N—C21—C13	123.0 (3)
C5—C4—C3	120.2 (3)	N—C21—H21	118.5
C5—C4—H4	119.9	C13—C21—H21	118.5
C3—C4—H4	119.9	C27—C22—C23	118.2 (3)
C4—C5—C6	120.9 (3)	C27—C22—N	117.6 (3)
C4—C5—H5	119.5	C23—C22—N	124.2 (3)
C6—C5—H5	119.5	C24—C23—C22	120.1 (3)
C7—C6—C5	122.8 (3)	C24—C23—H23	120.0
C7—C6—C1	117.9 (3)	C22—C23—H23	120.0
C5—C6—C1	119.3 (3)	C23—C24—C25	122.0 (3)
C8—C7—C6	122.0 (3)	C23—C24—H24	119.0
C8—C7—H7	119.0	C25—C24—H24	119.0
C6—C7—H7	119.0	C24—C25—C26	117.7 (3)
C7—C8—C9	120.4 (3)	C24—C25—C28	121.0 (3)
C7—C8—H8	119.8	C26—C25—C28	121.3 (3)
C9—C8—H8	119.8	C27—C26—C25	120.7 (3)
O1—C9—C10	119.6 (2)	C27—C26—H26	119.7
O1—C9—C8	120.7 (3)	C25—C26—H26	119.7
C10—C9—C8	119.8 (3)	C26—C27—C22	121.3 (3)
C9—C10—C1	120.1 (2)	C26—C27—H27	119.3
C9—C10—C11	120.1 (3)	C22—C27—H27	119.3
C1—C10—C11	119.7 (2)	C25—C28—H28A	109.5
C12—C11—C20	119.4 (2)	C25—C28—H28B	109.5
C12—C11—C10	120.8 (2)	H28A—C28—H28B	109.5
C20—C11—C10	119.8 (2)	C25—C28—H28C	109.5
O2—C12—C11	119.9 (2)	H28A—C28—H28C	109.5
O2—C12—C13	118.7 (2)	H28B—C28—H28C	109.5
C11—C12—C13	121.3 (2)	C29—O3—H3A	109.5
C14—C13—C21	118.8 (2)	O3—C29—C30	109.6 (4)
C14—C13—C12	119.0 (2)	O3—C29—H29A	109.7
C21—C13—C12	122.2 (3)	C30—C29—H29A	109.7
C13—C14—C15	121.3 (2)	O3—C29—H29B	109.7
C13—C14—H14	119.3	C30—C29—H29B	109.7
C15—C14—H14	119.3	H29A—C29—H29B	108.2

C14—C15—C16	120.9 (2)	C29—C30—H30A	109.5
C14—C15—C20	119.4 (2)	C29—C30—H30B	109.5
C16—C15—C20	119.7 (3)	H30A—C30—H30B	109.5
C17—C16—C15	121.0 (3)	C29—C30—H30C	109.5
C17—C16—H16	119.5	H30A—C30—H30C	109.5
C15—C16—H16	119.5	H30B—C30—H30C	109.5
C16—C17—C18	118.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3	0.82	1.95	2.753 (3)	164
O2—H2···N	0.80 (4)	1.90 (4)	2.612 (3)	148 (4)
O3—H3A···O2^{i}	0.82	2.08	2.844 (3)	155

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

Fig. 1

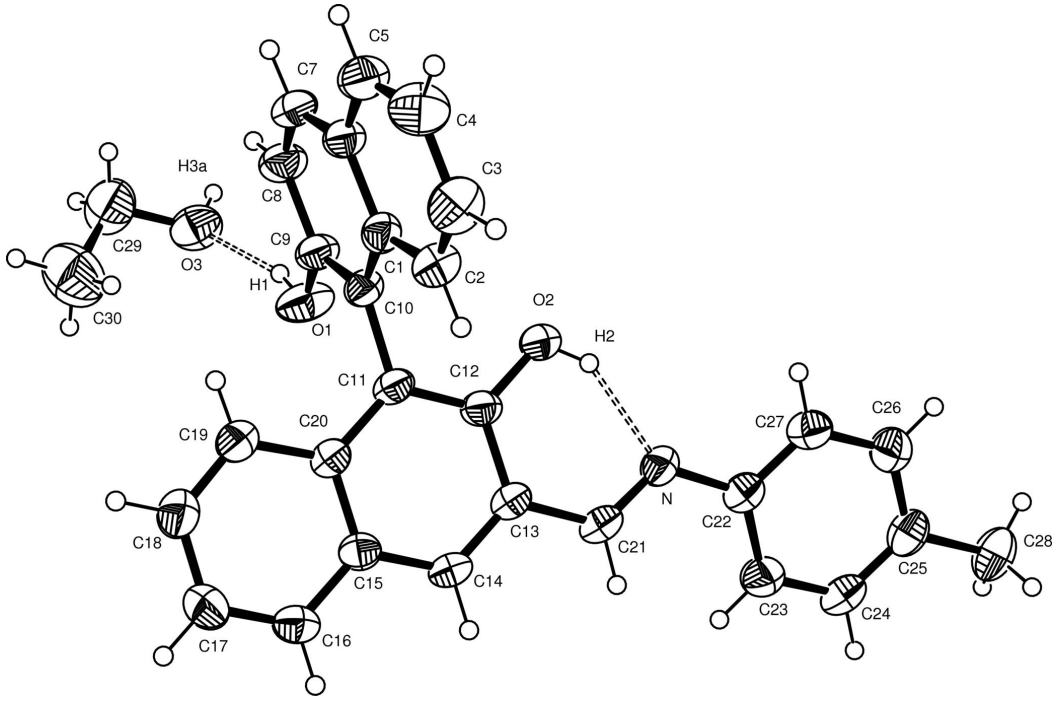

C5
C7
C4
H3a
C3
C8
C29
O3
C9
C1
C2
H1
C10
O1
C30
O2
H2
C11
C12
C19
C20
C27
C26
N
C22
C18
C13
C21
C28
C25
C15
C14
C23
C24
C17
C16

Fig. 2