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4-[2-(9-Anthryl)-2-hydroxyethyl]-4′-methyl-*trans*-2,2′-bipyridine: a ligand with 2,2′-bipyridine and anthracene subunits

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Key indicators

Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.001 Å
R factor = 0.054
wR factor = 0.157
Data-to-parameter ratio = 33.0

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

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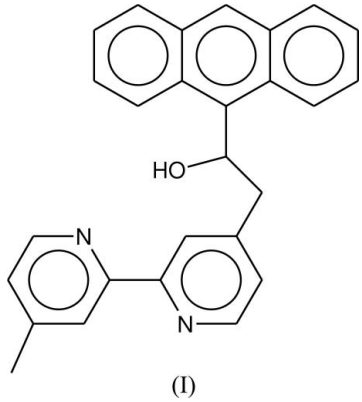
In the title compound, $C_{27}H_{22}N_2O$, the N—C—C—N torsion angle of the bipyridine unit has a magnitude of 171.21 (8)°, and the bipyridine and anthracene planes are approximately parallel, forming a dihedral angle of 6.24 (8)°. Molecules form centrosymmetric dimers *via* O—H···N hydrogen bonds of length 2.8221 (11) Å.

Comment

In studies of the photochemistry and photophysics of polypyridine–Ru complexes and their potential application in the photochemical decomposition of water, Cherry studied the effects of substituents on 2,2′-bipyridine ligands (Cherry & Henderson, 1984; Ollino & Cherry, 1985; Henderson *et al.*, 1984; Wacholtz *et al.*, 1985). The title compound, (I), was a product of that study, and the crystal structure determination has been carried out to confirm its identity.



(I)

The bipyridine is in the *anti* conformation, with an N1—C20—C22—N2 torsion angle of −171.21 (8)°, similar to that seen in 4,4′-dimethyl-2,2′-bipyridine, which lies on an inversion center (Beswick & Davies, 1996; Zhang *et al.*, 2003). The anthracene system is essentially planar, exhibiting a mean deviation of 0.014 Å for its 14C atoms, and a maximum deviation of 0.034 (1) Å for C12. The anthracene plane makes a dihedral angle of 6.24 (8)° with the mean plane of the 12 bipyridine non-H atoms.

Molecules form hydrogen-bonded dimers about inversion centers, with the distal N atom serving as acceptor, having graph-set descriptor (Etter, 1990) $R_2^2(18)$, as shown in Fig. 2.

Experimental

The compound was a gift from Professor William R. Cherry. Crystals were grown by evaporation of a methanol solution.

Crystal data

$C_{27}H_{22}N_2O$
$M_r = 390.47$
Triclinic, $P\overline{1}$
$a = 7.4985\ (10)$ Å
$b = 10.505\ (2)$ Å
$c = 12.782\ (2)$ Å
$\alpha = 82.102\ (9)^\circ$
$\beta = 73.795\ (10)^\circ$
$\gamma = 87.186\ (11)^\circ$
$V = 957.6\ (3)$ Å^3
$Z = 2$
$D_x = 1.354$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 110$ K
Parallelepiped, yellow
0.35 × 0.27 × 0.25 mm

Data collection

Nonius KappaCCD diffractometer with Oxford Cryostream
ω scans with κ offsets
Absorption correction: none
31964 measured reflections
9108 independent reflections
6314 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 36.3^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.157$
$S = 1.04$
9108 reflections
276 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 0.0951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H10H···N2^{i}	0.887 (17)	1.957 (17)	2.8221 (11)	164.7 (16)

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

For sp^2 C atoms, a C—H distance of 0.95 Å was used, and displacement parameters for H atoms were assigned as U_{iso}(H) = $1.2U_{eq}$ of the attached C atom. For the methyl group, C—H was set at 0.98 Å, U_{iso}(H) at $1.5U_{eq}$(C), and a torsional parameter was refined. The OH hydrogen was refined, with U_{iso}(H) = $1.5U_{eq}$(O).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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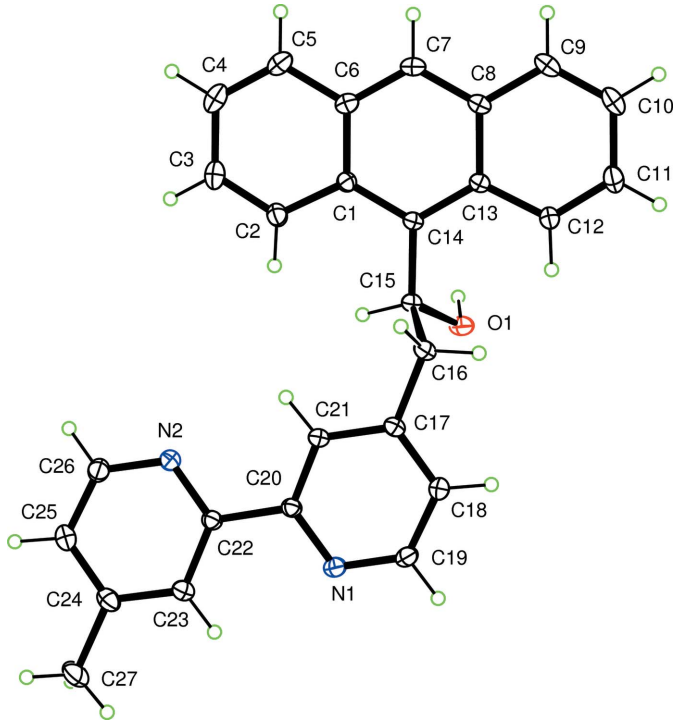

Figure 1
The title compound, showing the atom-numbering scheme, with displacement ellipsoids drawn at the 50% probability level.

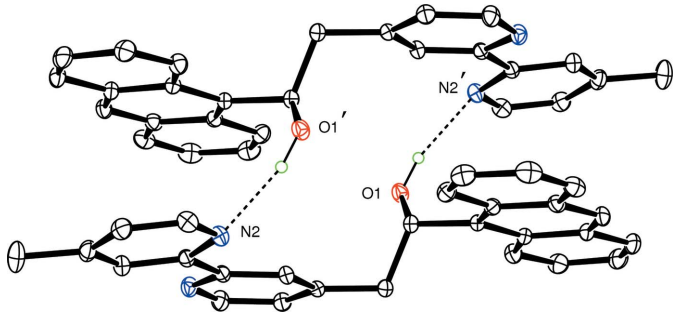

Figure 2
The hydrogen-bonded (dashed lines) dimer in (I). Only the OH H atoms are shown. The primed molecule is related by $(1-x, 1-y, 1-z)$.

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