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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.099
 wR factor = 0.176
Data-to-parameter ratio = 14.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Dicyclohexylammonium 1-(2-hydroxy-1-naphthyl)-2-naphtholate

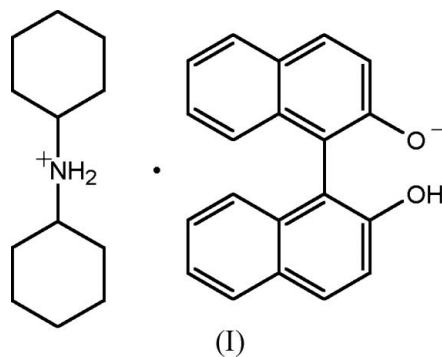
In the title compound, $\text{C}_{12}\text{H}_{24}\text{N}^+\cdot\text{C}_{20}\text{H}_{13}\text{O}_2^-$, the naphtholate anions are linked *via* an $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond, and are connected to the dicyclohexylammonium cations by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Received 26 September 2005

Accepted 11 October 2005

Online 15 October 2005

Comment

1,1'-Bi-2-naphthol (binaphthol) is usually used as a precursor for asymmetric catalysis (Pu, 1998), as a host for molecular recognition and enantiomer separation (Reeder *et al.*, 1994), and also as an intermediate for the synthesis of chiral materials (Zhang & Schuster, 1994). Many compounds of binaphthol have been studied previously (Periasamy *et al.*, 1997; Dobashi *et al.*, 1998; Lee *et al.*, 1999; Du *et al.*, 2002; Chandrasekhar *et al.*, 2003; Cheung *et al.*, 2003). Recently, the title compound, (I), has been obtained and its structure (Fig. 1) is discussed here.

Compound (I) consists of one dicyclohexylammonium cation and one 2-hydroxynaphthene-1-yl-2-naphtholate (NANAT) anion, where the binaphthol molecule loses a proton from one of the two hydroxyl groups. The $\text{C}12-\text{O}2$ bond length [1.317 (4) Å], where the O atom is anionic, is much shorter than the neutral $\text{C}2-\text{O}1$ bond [1.364 (4) Å]; this is consistent with the results of other studies (Goddard *et al.*, 2002; Sharma *et al.*, 2005). The two naphthalene ring systems are less twisted than those of binaphthol itself. This is indicated by the $\text{C}2-\text{C}1-\text{C}11-\text{C}12$ and $\text{C}10-\text{C}1-\text{C}11-\text{C}20$ torsion angles [-79.2 (4) and -77.0 (4)°, respectively], the absolute values of which are significantly smaller than those of binaphthol [88.3 (3) and 88.6 (3)°, respectively; Mori *et al.*, 1993].

In the crystal structure, the NANAT anions are linked *via* an $\text{O}1-\text{H}1\cdots\text{O}2^i$ hydrogen bond (symmetry codes as in Table 2), and are connected to the dicyclohexylammonium cations by $\text{N}1-\text{H}1\text{A}\cdots\text{O}2^i$, $\text{N}1-\text{H}1\text{B}\cdots\text{O}1^i$ and $\text{N}1-\text{H}1\text{B}\cdots\text{O}1^{ii}$ hydrogen bonds (Table 2 and Fig. 2).

Experimental

Binaphthol and dicyclohexylamine, in a molar ratio of 1:1, were mixed and dissolved in sufficient ethanol by heating to 353 K, to give a clear solution. Crystals of (I) were formed by gradual evaporation of ethanol over a period of one week at 293 K.

Crystal data

$C_{12}H_{24}N^+ \cdot C_{20}H_{13}O_2^-$
 $M_r = 467.63$
 Monoclinic, $P2_1/n$
 $a = 14.9935$ (11) Å
 $b = 10.1824$ (7) Å
 $c = 16.9848$ (12) Å
 $\beta = 98.434$ (2)°
 $V = 2565.0$ (3) Å³
 $Z = 4$

$D_x = 1.211$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1087 reflections
 $\theta = 2.5$ – 19.9°
 $\mu = 0.07$ mm⁻¹
 $T = 273$ (2) K
 Block, colourless
 $0.33 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.986$, $T_{max} = 0.991$
 13165 measured reflections

4533 independent reflections
 3102 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.049$
 $\theta_{max} = 25.0^\circ$
 $h = -13 \rightarrow 17$
 $k = -12 \rightarrow 11$
 $l = -20 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.099$
 $wR(F^2) = 0.176$
 $S = 1.21$
 4533 reflections
 317 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 1.412P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.16$ e Å⁻³
 $\Delta\rho_{min} = -0.16$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1–C2	1.364 (4)	C12–C13	1.426 (4)
O2–C12	1.317 (4)	N1–C27	1.501 (4)
C1–C2	1.366 (4)	N1–C21	1.503 (4)
C1–C11	1.497 (4)	C21–C22	1.508 (5)
C2–C1–C11	121.6 (3)	O2–C12–C11	122.3 (3)
C10–C1–C11	119.9 (3)	O2–C12–C13	120.0 (3)
O1–C2–C1	117.9 (3)	N1–C21–C22	107.7 (3)
O1–C2–C3	120.4 (3)		
C2–C1–C11–C12	−79.2 (4)	C10–C1–C11–C20	−77.0 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1 \cdots O2 ⁱ	0.82	1.80	2.510 (4)	144
N1–H1A \cdots O2 ⁱ	0.90	2.07	2.967 (4)	174
N1–H1B \cdots O1 ⁱ	0.90	2.23	2.841 (4)	125
N1–H1B \cdots O2 ⁱⁱ	0.90	2.48	3.366 (5)	168

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

All H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances of N–H = 0.90, O–H = 0.82 and C–H = 0.93 (aromatic), 0.97 (methylene) or 0.98 Å (methine), with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(\text{parent atom})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve

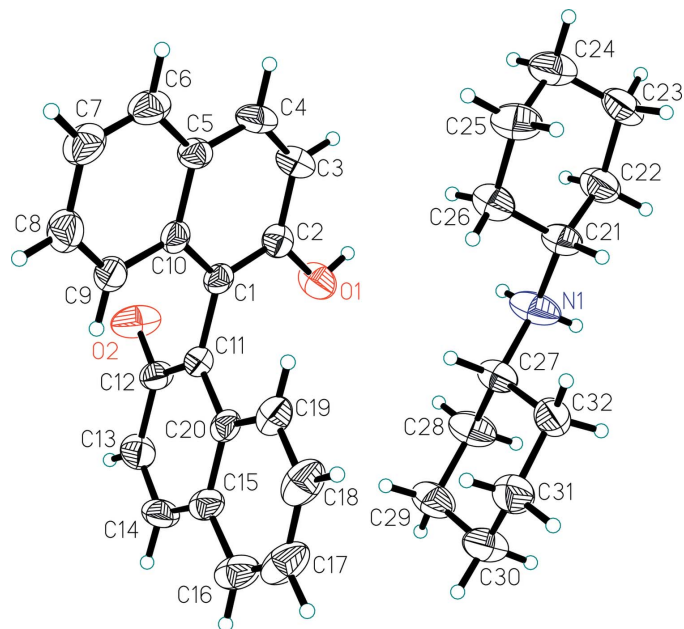


Figure 1

A view of (I), with the atom-numbering scheme and 40% probability displacement ellipsoids.

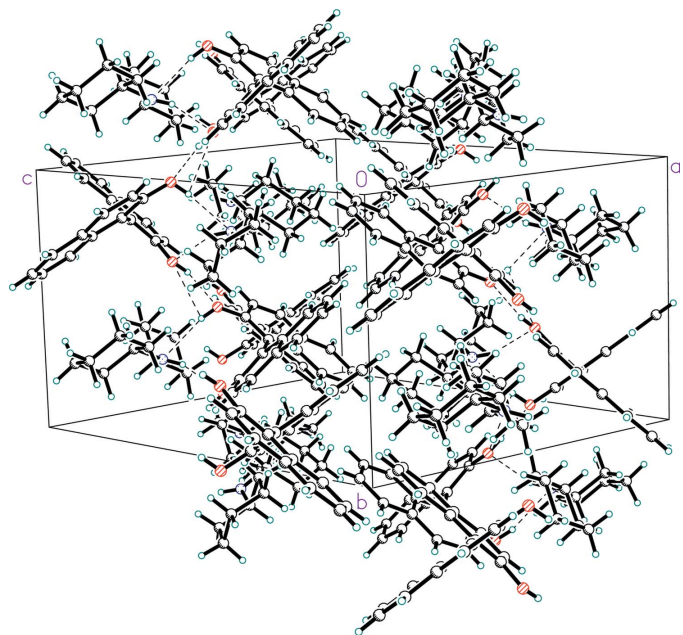


Figure 2

A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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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