O(3)	0.5368 (7)	0.6593 (8)	0.8832 (7)	0.057 (3)
C(4)	0.6318 (10)	0.5817 (11)	0.7968 (10)	0.039 (3)
O(1)	1.1920 (7)	0.6483 (9)	0.8257 (8)	0.062 (3)
C(1)	1.1344 (10)	0.5666 (11)	0.7283 (10)	0.039 (3)
O(2)	1.2303 (8)	0.4818 (9)	0.6476 (7)	0.053 (3)

Table 2. *Bond lengths* (Å) *and angles* (°)

Br(1)—C(2)	1.975 (9)	O(4)—C(4)	1.22 (1)
C(2)—C(3)	1.52 (1)	C(2)—C(1)	1.52 (1)
C(3)—C(4)	1.51 (1)	O(3)—C(4)	1.28 (1)
O(1)—C(1)	1.25 (1)	C(1)—O(2)	1.28 (1)
Br(1)—C(2)—C(3)	109.3 (6)	Br(1)—C(2)—C(1)	102.9 (6)
C(3)—C(2)—C(1)	111.8 (7)	C(2)—C(3)—C(4)	112.0 (7)
O(4)—C(4)—C(3)	121.9 (8)	O(4)—C(4)—O(3)	124.5 (7)
C(3)—C(4)—O(3)	113.6 (8)	C(2)—C(1)—O(1)	121.3 (8)
C(2)—C(1)—O(2)	114.2 (8)	O(1)—C(1)—O(2)	124.5 (7)

Reflections were corrected for crystal decay. The structure was solved by direct methods. Reflections in the range $-3\sigma_I \leq I \leq 3\sigma_I$ [$\sigma_I = (N_p + N_b)^{1/2}$, where N_p is the number of counts in the peak and N_b is the number of counts in the background] were treated by the method of French & Wilson (1978). Reflections with $k = 6$ were not used in refinement because the crystal was twinned and the twin interfered with this layer. H atoms were placed in calculated positions, with fixed temperature factors, and were constrained to ride on the atoms to which they were attached. Anomalous-dispersion corrections were applied to N, O and Br atoms. Calculations were made using *SHELXTL PC* (Sheldrick, 1990) and Laser386 or IBM486 computers.

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Lists of structure factors, anisotropic thermal parameters, H-atom positional parameters and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55932 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: BR1027]

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(+)-(*R*)- and Racemic Forms of 2,2′-Dihydroxy-1,1′-binaphthyl

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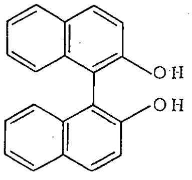
Abstract

The molecules of 1,1′-binaphthyl-2,2′-diol, related by a 3_1 axis in the (+)-(*R*) form and by a 2_1 axis in the racemic form, are linked through hydrogen bonds between the hydroxyl groups. The dihedral angles between the planes of the naphthyl groups are close to 90° for the molecules in both crystals: 101.65 (5)° in the (+)-(*R*) form and 90.58 (4)° in the racemic form.

Comment

Optical isomers exist for the title compound (I) because of steric hindrance around the C(sp^2)—C(sp^2) bond between the naphthyl groups (Akimoto, Shioiri, Iitaka & Yamada, 1968). The present work has been carried out in order to determine the molecular conformation, the mode of hydrogen bonding and the relationship between the molecular arrangements in the crystals of the (+)-(*R*) and racemic forms which were formed from toluene and ethanol solutions, respectively, by slow evaporation. For the latter form, the atomic parameters of the non-H atoms have been reported (Gridunova, Furmanova, Shklover, Struchkov, Ezhkova & Chayanov, 1982), but the H-atom positions to specify the hydrogen bonding have not been determined.



(I)

Corresponding bond lengths and angles in both forms of the crystals are in agreement within their e.s.d.'s. Corresponding bond lengths and angles of the two naphthyl groups in each molecule are substantially the same. In both crystals, C(1)—C(2)

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bonds are longer than C(3)—C(4) as found in racemic and optically active forms of 1,1′-binaphthyl (Kress, Duesler, Etter, Paul & Curtin, 1980) and other 1,1′-binaphthyl derivatives: 4,4′-diamino-1,1′-binaphthyl (Pauptit & Trotter, 1983), (−)-2,2′-bisbromomethyl-1,1′-binaphthyl (Harata & Tanaka, 1973), (+)-2,2-dihydroxy-1,1′-binaphthalene-3,3′-dicarboxylic acid dimethyl ester (Akimoto & Iitaka, 1969), and optically active 4,4′-dimethyl-1,1′-binaphthyl (Pauptit & Trotter, 1981).

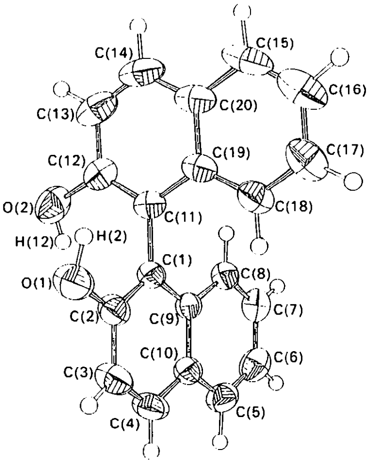

Fig. 1. The thermal ellipsoids with atomic numbering. Ellipsoids of 50% probability are drawn for the non-H atoms of the (+)-(*R*) form; the H atoms are represented as spheres equivalent to $B = 1.0$ Å^2.

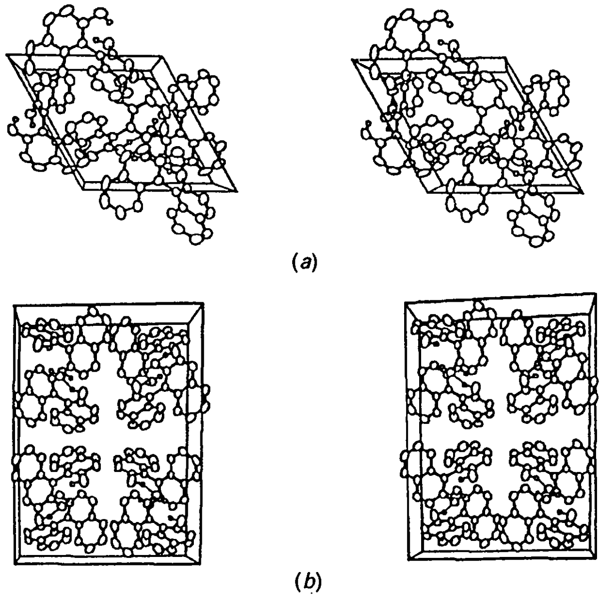

Fig. 2. Stereoscopic view of the crystal structures viewed down the *c* axes. The intermolecular hydrogen bonds are shown by thin lines. (*a*) The (+)-(*R*) form; the *b* axis points upwards and the *a* axis from left to right. (*b*) The racemic form; the *b* axis points upwards and the *a* axis from left to right.

The torsion angle χ[C(2)—C(1)—C(11)—C(19)] is 99.2 (3)° in the (+)-(*R*) form and 88.6 (3)° in the racemic form. According to *MM*2 calculations (Allinger & Yuh, 1985), the steric energy at the observed conformation is higher than the minimum energy at $\chi = 90°$ by only 0.59 kJ mol^{-1} in the (+)-(*R*) form and by 0.04 kJ mol^{-1} in the racemic form.

In both crystals, angles C(1)—C(2)—O(1) and C(11)—C(12)—O(2) are larger than the sp^2 angles because of the steric repulsions O(1)···C(11) and O(2)···C(1), respectively [2.855 (4) and 2.873 (3) Å in the (+)-(*R*) form, 2.873 (3) and 2.859 (4) Å in the racemic form].

In the (+)-(*R*) form, the intermolecular hydrogen bonding is formed around a 3_1 axis [O(1)···O(2) 2.961 (4), H(2)···O(2) 2.11 (4) Å, O(1)—H(2)···O(2) 152 (3)°], while in the racemic form the hydrogen bonding is formed around a 2_1 axis [O(1)···O(2) 2.852 (3), H(2)···O(2) 2.03 (4) Å, O(1)—H(2)···O(2) 141 (3)°]. Thus, the crystal structures of both forms are totally different from each other.

Experimental

(+)-(*R*) form

Crystal data

$C_{20}H_{14}O_2$
$M_r = 286.33$
Trigonal
$P3_1$
$a = 10.808\ (2)$ Å
$c = 10.883\ (1)$ Å
$V = 1101.0\ (4)$ Å^3
$Z = 3$
$D_x = 1.295$ Mg m^{-3}
$D_m = 1.30$ Mg m^{-3}
Density measured by flotation in aqueous KI

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 20 reflections
$\theta = 19\text{–}20°$
$\mu = 0.621$ mm^{-1}
$T = 295$ K
Prism elongated along *c*
0.38 × 0.30 × 0.25 mm
Colourless
Crystal source: recrystallized from toluene solution, TCI EP B1142

Data collection

Rigaku AFC-5 diffractometer
ω-2θ scans; width $1.2 + 0.15\tan\theta)°$ in ω; rate 4° min^{-1} in ω; background counts 4 s on each side of every scan
Absorption correction: none
1266 measured reflections
1091 independent reflections

1077 observed reflections $[F > 1.0\sigma(F)]$
$R_{\rm int} = 0.02$
$\theta_{\rm max} = 60.0°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 12$
$l = -12 \rightarrow 12$
3 standard reflections monitored every 97 reflections intensity variation: 1.2%

Refinement

Refinement on *F*
Final $R = 0.03$
$wR = 0.039$

$(\Delta/\sigma)_{\rm max} = 0.05$
$\Delta\rho_{\rm max} = 0.09$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.13$ e Å^{-3}

$S = 1.357$
1077 reflections
258 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) - 0.0017|F_o| + 0.009|F_o|^2]$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Racemic form

Crystal data

$C_{20}H_{14}O_2$
$M_r = 286.33$
Orthorhombic
*Iba*2
$a = 15.696$ (2) Å
$b = 21.617$ (2) Å
$c = 8.6253$ (6) Å
$V = 2926.6$ (4) Å^3
$Z = 8$
$D_x = 1.300$ Mg m^{-3}
$D_m = 1.30$ Mg m^{-3}
Density measured by flotation in aqueous KI

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 20 reflections
$\theta = 19\text{–}21°$
$\mu = 0.623$ mm^{-1}
$T = 295$ K
Plate developed {010}
0.25 × 0.20 × 0.10 mm
Colourless
Crystal source: recrystallized from ethanol solution, TC EP B0461

Data collection

Rigaku AFC-5 diffractometer
ω-2θ scans; width 1.2 + 0.15tanθ)° in ω; rate 4° min^{-1} in ω; background counts 4 s on each side of every scan
Absorption correction: none
1358 measured reflections
1258 independent reflections

1197 observed reflections $[F > 1.0\sigma(F)]$
$R_{\text{int}} = 0.020$
$\theta_{\max} = 62.5°$
$h = -1 \rightarrow 18$
$k = 0 \rightarrow 24$
$l = 0 \rightarrow 9$
3 standard reflections monitored every 97 reflections intensity variation: 0.8%

Refinement

Refinement on F
Final $R = 0.034$
$wR = 0.039$
$S = 1.214$
1197 reflections
258 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) - 0.0340|F_o| + 0.0042|F_o|^2]$

$(\Delta/\sigma)_{\max} = 0.19$
$\Delta\rho_{\max} = 0.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{\text{eq}} = \tfrac{4}{3}\Sigma_i\beta_{ii}/a_i^{*2}.$$

	x	y	z	B_{eq}
(+)-(*R*) form				
O(1)	0.4028 (2)	0.2926 (2)	0.5348 (2)	4.75 (8)
O(2)	0.5488 (2)	0.2585 (2)	0.8018 (2)	5.84 (9)
C(1)	0.3997 (2)	0.4035 (2)	0.7263 (2)	3.16 (8)
C(2)	0.3311 (2)	0.3150 (2)	0.6274 (2)	3.57 (9)
C(3)	0.1810 (3)	0.2431 (3)	0.6169 (3)	4.3 (1)
C(4)	0.1017 (2)	0.2608 (3)	0.7033 (3)	4.0 (1)
C(5)	0.0834 (3)	0.3741 (3)	0.8953 (3)	4.5 (1)
C(6)	0.1477 (3)	0.4660 (3)	0.9899 (3)	5.1 (1)
C(7)	0.2967 (3)	0.5395 (3)	1.0015 (2)	4.6 (1)
C(8)	0.3794 (2)	0.5200 (2)	0.9167 (2)	3.66 (9)
C(9)	0.3167 (2)	0.4253 (2)	0.8164 (2)	3.15 (8)
C(10)	0.1655 (2)	0.3527 (2)	0.8052 (2)	3.47 (9)
C(11)	0.5588 (2)	0.4762 (2)	0.7343 (2)	3.37 (9)
C(12)	0.6243 (3)	0.4007 (3)	0.7708 (2)	4.3 (1)
C(13)	0.7743 (3)	0.4660 (4)	0.7752 (3)	6.1 (1)
C(14)	0.8571 (3)	0.6036 (4)	0.7397 (3)	5.4 (1)
C(15)	0.8792 (3)	0.8290 (3)	0.6520 (3)	4.6 (1)
C(16)	0.8161 (3)	0.9024 (3)	0.6122 (3)	5.0 (1)
C(17)	0.6688 (3)	0.8411 (3)	0.6165 (3)	5.0 (1)
C(18)	0.5856 (3)	0.7040 (3)	0.6566 (2)	3.9 (1)
C(19)	0.6447 (2)	0.6211 (3)	0.6971 (2)	3.37 (9)
C(20)	0.7964 (2)	0.6857 (3)	0.6973 (2)	4.0 (1)
Racemic form				
O(1)	0.1326 (1)	0.17199 (9)	0.8636 (2)	5.47 (9)
O(2)	0.2450 (1)	0.27154 (8)	0.5628 (2)	4.48 (8)
C(1)	0.2123 (1)	0.1446 (1)	0.6346 (3)	3.08 (9)
C(2)	0.1396 (1)	0.1439 (1)	0.7218 (3)	3.7 (1)
C(3)	0.0654 (1)	0.1137 (1)	0.6703 (3)	4.3 (1)
C(4)	0.0656 (1)	0.0829 (1)	0.5336 (3)	4.2 (1)
C(5)	0.1413 (2)	0.0496 (1)	0.2942 (4)	4.8 (1)
C(6)	0.2114 (2)	0.0510 (1)	0.2038 (4)	5.9 (2)
C(7)	0.2840 (2)	0.0839 (2)	0.2518 (4)	5.7 (1)
C(8)	0.2850 (1)	0.1136 (1)	0.3904 (4)	4.4 (1)
C(9)	0.2133 (1)	0.1132 (1)	0.4885 (3)	3.35 (9)
C(10)	0.1397 (1)	0.0809 (1)	0.4385 (3)	3.6 (1)
C(11)	0.2894 (1)	0.1785 (1)	0.6925 (3)	2.97 (9)
C(12)	0.2997 (1)	0.2401 (1)	0.6591 (3)	3.36 (9)
C(13)	0.3672 (1)	0.2752 (1)	0.7215 (3)	4.0 (1)
C(14)	0.4243 (1)	0.2484 (1)	0.8165 (3)	4.1 (1)
C(15)	0.4783 (1)	0.1548 (1)	0.9519 (3)	4.3 (1)
C(16)	0.4733 (2)	0.0931 (1)	0.9815 (3)	5.0 (1)
C(17)	0.4083 (2)	0.0577 (1)	0.9140 (3)	4.8 (1)
C(18)	0.3482 (1)	0.0848 (1)	0.8222 (3)	3.9 (1)
C(19)	0.3512 (1)	0.1489 (1)	0.7892 (3)	3.19 (9)
C(20)	0.4194 (1)	0.1842 (1)	0.8531 (3)	3.49 (9)

Table 2. *Geometric parameters* (Å, °)

	(+)-(*R*) form	Racemic form
O(1)—C(2)	1.365 (4)	1.370 (4)
O(2)—C(12)	1.374 (4)	1.374 (4)
C(1)—C(2)	1.383 (4)	1.367 (4)
C(1)—C(9)	1.426 (3)	1.431 (4)
C(1)—C(11)	1.494 (4)	1.500 (4)
C(2)—C(3)	1.411 (4)	1.407 (4)
C(3)—C(4)	1.349 (4)	1.354 (4)
C(4)—C(10)	1.417 (4)	1.419 (4)
C(5)—C(6)	1.356 (4)	1.349 (4)
C(5)—C(10)	1.417 (4)	1.417 (4)
C(6)—C(7)	1.400 (4)	1.405 (4)
C(7)—C(8)	1.373 (4)	1.357 (4)
C(8)—C(9)	1.416 (4)	1.408 (4)
C(9)—C(10)	1.421 (3)	1.422 (4)
C(11)—C(12)	1.380 (4)	1.372 (4)
C(11)—C(19)	1.422 (4)	1.430 (4)
C(12)—C(13)	1.408 (5)	1.410 (4)
C(13)—C(14)	1.353 (6)	1.345 (4)
C(14)—C(20)	1.419 (5)	1.425 (4)
C(15)—C(16)	1.350 (6)	1.360 (4)
C(15)—C(20)	1.434 (5)	1.409 (4)
C(16)—C(17)	1.386 (5)	1.402 (4)
C(17)—C(18)	1.365 (4)	1.364 (4)
C(18)—C(19)	1.406 (4)	1.415 (4)
C(19)—C(20)	1.425 (4)	1.425 (4)
O(1)—H(2)	0.93 (4)	0.97 (4)
O(2)—H(12)	0.83 (3)	0.94 (3)
C(2)—C(1)—C(9)	119.0 (2)	119.2 (3)
C(2)—C(1)—C(11)	119.1 (2)	119.7 (3)
C(9)—C(1)—C(11)	121.8 (2)	121.0 (3)
O(1)—C(2)—C(1)	122.8 (3)	123.6 (3)
O(1)—C(2)—C(3)	116.2 (3)	114.9 (3)
C(1)—C(2)—C(3)	121.0 (3)	121.5 (3)
C(2)—C(3)—C(4)	120.2 (3)	120.1 (3)
C(3)—C(4)—C(10)	121.6 (3)	121.3 (3)
C(6)—C(5)—C(10)	120.7 (3)	120.9 (3)
C(5)—C(6)—C(7)	120.5 (3)	120.2 (3)

C(6)—C(7)—C(8)	120.3 (3)	120.5 (3)
C(7)—C(8)—C(9)	121.1 (3)	121.1 (3)
C(1)—C(9)—C(8)	122.4 (2)	122.3 (3)
C(1)—C(9)—C(10)	119.6 (2)	119.4 (3)
C(8)—C(9)—C(10)	117.9 (2)	118.3 (3)
C(4)—C(10)—C(5)	122.1 (2)	122.7 (3)
C(4)—C(10)—C(9)	118.5 (2)	118.4 (3)
C(5)—C(10)—C(9)	119.5 (2)	118.9 (3)
C(1)—C(11)—C(12)	120.1 (3)	119.9 (2)
C(1)—C(11)—C(19)	120.6 (3)	121.5 (2)
C(12)—C(11)—C(19)	119.2 (3)	118.5 (2)
O(2)—C(12)—C(11)	122.6 (3)	122.2 (3)
O(2)—C(12)—C(13)	116.3 (3)	115.7 (3)
C(11)—C(12)—C(13)	121.1 (3)	122.1 (3)
C(12)—C(13)—C(14)	120.2 (4)	120.1 (3)
C(13)—C(14)—C(20)	121.5 (4)	121.2 (3)
C(16)—C(15)—C(20)	121.2 (4)	121.2 (3)
C(15)—C(16)—C(17)	120.4 (4)	119.9 (3)
C(16)—C(17)—C(18)	120.3 (3)	120.7 (3)
C(17)—C(18)—C(19)	122.0 (3)	121.0 (3)
C(11)—C(19)—C(18)	122.4 (3)	122.2 (3)
C(11)—C(19)—C(20)	119.8 (3)	119.7 (2)
C(18)—C(19)—C(20)	117.8 (3)	118.1 (3)
C(14)—C(20)—C(15)	123.6 (3)	122.5 (2)
C(14)—C(20)—C(19)	118.2 (3)	118.4 (2)
C(15)—C(20)—C(19)	118.2 (3)	119.0 (2)
C(2)—O(1)—H(2)	111 (3)	106 (2)
C(12)—O(2)—H(12)	106 (2)	115 (2)

Data collection and cell refinement: Rigaku AFC-5 software (1977). Data reduction: *NTDATAIN* (Tanaka, 1979). Program used to solve structure: *MULTAN*11/84 (Main, Germain & Woolfson, 1984). Programs used to refine structure (block-diagonal least squares): *HBLS*-V and *DAPH* (Ashida, 1973). Software used to prepare material for publication: *MOLCON* (Fujii, 1979); *ORTEP*II (Johnson, 1971). Computations were carried out at the Research Center for Protein Engineering, Institute for Protein Research, Osaka University, and at the Okayama University Computer Center.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55956 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1012]

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Structure of 6-*O*-Methylerythromycin A (Clarithromycin)

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Abstract

The absolute configuration of the asymmetric centers in clarithromycin is the same as that in erythromycin A [Harris, McGeachin & Mills (1965). *Tetrahedron Lett.* pp. 679–685; Oliver & Strickland (1986). *Acta Cryst.* **C42**, 952–956]. The molecular structure is similar to that of erythromycin A. The carbonyl and the hydroxyl groups of the 14-membered aglycone are on the same side of the aglycone ring, and the 6-*O*-methyl group is in this hydrophilic region.

Comment

Clarithromycin, (I), a new semisynthetic macrolide antibiotic, has been clinically used for the treatment of infectious diseases caused by aerobic gram-positive bacteria, some gram-negative bacteria, anaerobic bacteria, *Mycoplasma* and *Chlamydia.* This antibiotic shows a similar antibacterial spectrum to erythromycin A, and its activity is twofold higher than that of erythromycin A *in vitro.* It exhibits much higher *in vivo* activity than erythromycin A because of its superior pharmacokinetic properties (Morimoto, Misawa, Adachi, Nagate, Watanabe & Omura, 1990; Morimoto, Nagate,

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