standard deviation of the non-hydrogen atoms from the least-squares plane is 0·014 Å. The dimensions of hydroquinone are also similar to those found in several other crystal structures (Mahmoud & Wallwork, 1975). The significant difference between C(6)–C(5)–O(1) and C(7)–C(5)–O(1) is in accord with the observation that, for many phenols, the C–C–OH angle is somewhat larger on the side of the H atom (Mahmoud & Wallwork, 1975).

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1-Methyl-2-naphthyl Acetate

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Abstract. $C_{13}H_{12}O_2$, monoclinic, $P2_1/c$, $Z = 4$, $M_r = 200$, $a = 6·46$, $b = 8·33$, $c = 20·25$ Å, $\beta = 91·90°$, $U = 1088$ Å^3, $D_m = 1·41$, $D_x = 1·22$ g cm^{-3}, $\lambda = 0·7107$ Å, μ(Mo $K\alpha$) = 0·88 cm^{-1}, $F(000) = 424$, $R = 4·6$%. The molecular dimensions in the aromatic system are similar to those in naphthalene itself.

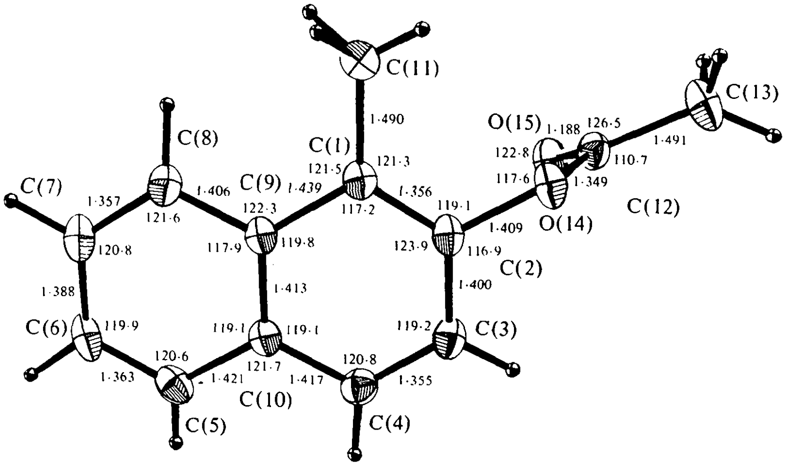

Fig. 1. A view of the molecule, showing bond lengths (Å) and bond angles (°).

Introduction. Cell dimensions were initially determined from precession photographs and subsequently adjusted to minimize the discrepancies between calculated and observed setting angles measured on a Hilger & Watts Y290 four-circle computer-controlled diffractometer. The systematic absences, 0*k*0 when $k = 2n + 1$ and *h*0*l* when $l = 2n + 1$, determine the space group as $P2_1/c$. The intensities were obtained by the ω–2θ step-scan procedure (40 steps of 0·02°) with background intensity measurements at each end of the scan range (counting times: scan 1 s/step; background 20 s) and periodic monitoring of two standard reflexions. 1682 intensities ($2\theta \leq 52°$) with $I \geq 2\sigma(I)$ were obtained by irradiating a crystal 1 × 1 × 1 mm with Mo $K\alpha$ radiation.

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses*

	x	*y*	*z*
C(1)	5324 (3)	779 (2)	1196 (1)
C(2)	4623 (3)	1732 (2)	693 (1)
C(3)	2786 (3)	2624 (2)	705 (1)
C(4)	1639 (3)	2581 (2)	1253 (1)
C(5)	1146 (4)	1637 (3)	2398 (1)
C(6)	1824 (4)	766 (3)	2933 (1)
C(7)	3635 (4)	−127 (3)	2903 (1)
C(8)	4743 (4)	−150 (2)	2346 (1)
C(9)	4134 (3)	752 (2)	1784 (1)
C(10)	2288 (3)	1658 (2)	1810 (1)
C(11)	7228 (4)	−215 (3)	1137 (1)
C(12)	6982 (3)	3031 (2)	6 (1)
C(13)	7935 (6)	2922 (4)	−653 (1)
O(14)	5717 (2)	1770 (2)	102 (1)
O(15)	7262 (2)	4061 (2)	405 (1)
H(3)	2445 (30)	3273 (25)	338 (10)
H(4)	344 (36)	3142 (27)	1287 (10)
H(5)	−98 (37)	2208 (29)	2391 (11)
H(6)	1038 (35)	785 (27)	3324 (12)
H(7)	4176 (37)	−722 (29)	3296 (13)
H(8)	6064 (40)	−748 (31)	2325 (12)
H(111)	8170 (46)	−41 (35)	1474 (15)
H(112)	7885 (37)	−55 (28)	720 (13)
H(113)	6816 (48)	−1414 (38)	1180 (14)
H(131)	8219 (47)	1878 (42)	−761 (14)
H(132)	9153 (68)	3526 (50)	−656 (19)
H(133)	6932 (60)	3298 (45)	−976 (19)

The coordinates of all the nonhydrogen atoms were obtained with *MULTAN*. Subsequent full-matrix least-squares calculations with the 1508 reflexions for which $|F_o| \geq 7\sigma(|F_o|)$, anisotropic thermal parameters for C and O, and isotropic parameters for the H atoms, located in a difference map towards the end of refinement, converged at $R = 4·6\%$.[*] A weighting scheme $w = 1/(A + B|F_o| + C|F_o|^2)$ with $A = 0·1728$, $B = -0·0277$ and $C = 0·0350$ was applied and no correction was made for absorption. Fractional atomic coordinates are given in Table 1. Bond lengths and angles are in Fig. 1.

Discussion. It has been reported that the rate at which 1-alkyl-2-naphthols react with oxygen to give hydroperoxides increases as the expected steric strain in the alkylnaphthol is increased (Brady & Carnduff, 1974). Thus, while 1-methyl-2-naphthol and 1-methyl-6-*tert*-butyl-2-naphthol are essentially inert under the conditions used, 1-isopropyl- and 1,8-dimethyl-2-naphthol react in a few hours and the 1-*tert*-butyl compound in a few minutes. One possible explanation would be that there is some release of *peri* strain consequent upon the formation of a C(1)-tetrahedral intermediate, which might contribute to a reduction in the activation energy for a rate-limiting step in the free-radical autoxidation. Since the alkylnaphthols are unstable in air, X-ray

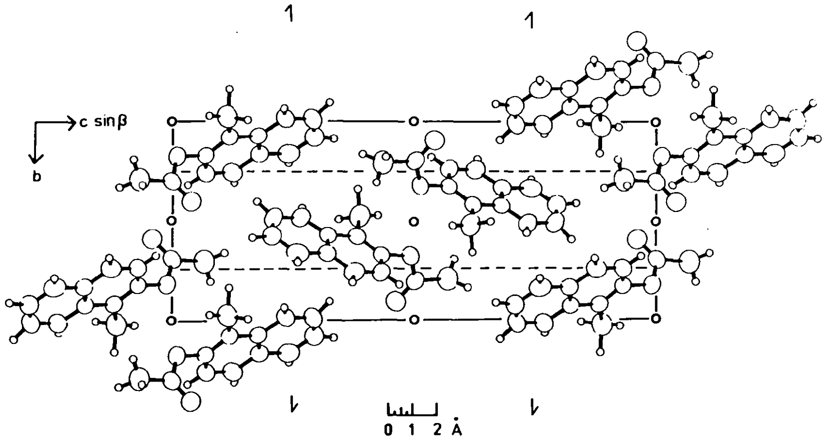

Fig. 2. The crystal packing.

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[*] Lists of structure factors, anisotropic thermal parameters and details of the complete molecular geometry have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32765 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

crystal structure analyses have been performed on the acetates of a number of 1-alkyl-2-naphthols in order to obtain quantitative estimates of the strain present.

As expected, there is no evidence of significant *peri* strain in 1-methyl-2-naphthol and the molecular geometry is unexceptional.* The only noteworthy difference between the aromatic systems of naphthalene (Pawley & Yeats, 1969) and 1-methyl-2-naphthol is the C(1)—C(9)—C(8) angle of 120·2° in the former and 122·3° in the latter. The opening out of this valency angle is a very effective way of moving H(8) and the H atoms on C(11) out of close proximity.

The crystal packing is shown in Fig. 2.

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* See previous footnote.

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1-Isopropyl-2-naphthyl Acetate

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Abstract. $C_{15}H_{16}O_2$, orthorhombic, *Pbca*, $Z = 8$, $M_r = 228$, $a = 19·17$, $b = 8·59$, $c = 15·46$ Å, $U = 2546$ Å^3, $D_m = 1·07$, $D_x = 1·19$ g cm^{-3}, $\lambda = 0·7107$ Å, μ(Mo $K\alpha$) = 0·84 cm^{-1}, $F(000) = 976$, $R = 6·1\%$. An additional increase in the C(1)—C(9)—C(8) angle results from the replacement of a methyl by the ispropyl group.

Introduction. The data collection and structure determination were identical to those for 1-methyl-2-naphthyl acetate, with the following exceptions: the systematic absences are $h0l$ when $l = 2n + 1$, $hk0$ when $h = 2n + 1$ and $0kl$ when $k = 2n + 1$; peaks were scanned in 80 steps of 0·01° at 1·5 s/step with two 30 s background counts. 2234 ($2\theta \leq 40°$) intensities were measured; the crystal size was 1 × 1 × 0·3 mm. Least-squares refinement was carried out with the 1155 structure amplitudes for which $|F_o| \geq 4\sigma(|F_o|)$ and convergence was obtained at $R = \Sigma(|F_o| - |F_c|)/\Sigma|F_o| = 6·1\%$.* The weighting scheme was $w = 1/(A + B|F_o| + C|F_o|^2)$ with $A = 0·4999$, B $-0·3020$ and $C = 0·0049$. The fractional atomic coordinates are given in Table 1.

Table 1. *Fractional atomic coordinates* (×10^4) *with e.s.d.'s in parentheses*

	x	*y*	*z*
C(1)	1432 (3)	8663 (5)	2290 (3)
C(2)	908 (3)	8983 (6)	1715 (3)
C(3)	469 (3)	10296 (6)	1763 (3)
C(4)	562 (3)	11325 (6)	2412 (4)
C(5)	1163 (3)	12127 (6)	3755 (4)
C(6)	1646 (3)	11869 (7)	4372 (3)
C(7)	2088 (3)	10589 (7)	4314 (4)
C(8)	2029 (3)	9574 (6)	3648 (3)
C(9)	1518 (3)	9745 (6)	2988 (3)
C(10)	1083 (3)	11088 (6)	3049 (3)
C(11)	1879 (2)	7193 (6)	2222 (3)
C(12)	740 (3)	8276 (7)	231 (3)
C(13)	470 (3)	6950 (7)	−301 (3)
C(17)	1455 (4)	5729 (7)	2396 (5)
C(18)	2274 (3)	7090 (7)	1374 (4)
O(14)	744 (2)	7858 (4)	1083 (2)
O(15)	929 (2)	9496 (5)	−26 (3)
H(3)	114 (26)	10370 (61)	1253 (32)
H(4)	266 (24)	12342 (61)	2424 (31)
H(5)	855 (23)	13030 (53)	3719 (30)
H(6)	1686 (24)	12616 (61)	4874 (29)
H(7)	2421 (24)	10459 (51)	4729 (26)
H(8)	2325 (20)	8747 (49)	3601 (25)
H(11)	2265 (27)	7276 (65)	2686 (33)
H(131)	534 (37)	7043 (92)	−963 (48)
H(132)	−24 (31)	6946 (66)	−308 (36)
H(133)	670 (41)	6045 (79)	−150 (48)
H(171)	1750 (26)	4924 (58)	2401 (33)
H(172)	1229 (38)	5782 (88)	2949 (54)
H(173)	1067 (33)	5577 (76)	1932 (42)
H(181)	2663 (26)	6283 (64)	1419 (31)
H(182)	2494 (28)	7935 (62)	1210 (34)
H(183)	1936 (42)	6796 (84)	877 (44)

Discussion. Fig. 1 shows that there has been a further

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* Lists of structure factors, anisotropic thermal parameters and details of the complete molecular geometry have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32766 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.