

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

\* See previous footnote.

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.

### References

- BRADY, P. A. & CARNDUFF, J. (1974). *Chem. Commun.* pp. 816–817.  
 PAWLEY, G. S. & YEATS, E. A. (1969). *Acta Cryst.* B25, 2009–2013.

*Acta Cryst.* (1977). B33, 2984–2985

## 1-Isopropyl-2-naphthyl Acetate

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(Received 19 May 1977; accepted 4 June 1977)

**Abstract.** C<sub>15</sub>H<sub>16</sub>O<sub>2</sub>, orthorhombic, *Pbca*, *Z* = 8, *M<sub>r</sub>* = 228, *a* = 19.17, *b* = 8.59, *c* = 15.46 Å, *U* = 2546 Å<sup>3</sup>, *D<sub>m</sub>* = 1.07, *D<sub>x</sub>* = 1.19 g cm<sup>-3</sup>, *λ* = 0.7107 Å, *μ*(Mo *Kα*) = 0.84 cm<sup>-1</sup>, *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 isopropyl 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 *h*0*l* when *l* = 2*n* + 1, *hk*0 when *h* = 2*n* + 1 and 0*kl* when *k* = 2*n* + 1; peaks were scanned in 80 steps of 0.01° at 1.5 s/step with two 30 s background counts. 2234 (2θ ≤ 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<sub>o</sub>*| ≥ 4σ(|*F<sub>o</sub>*|) and convergence was obtained at *R* = Σ(|*F<sub>o</sub>*| – |*F<sub>c</sub>*|)/Σ |*F<sub>o</sub>*| = 6.1%.\* The weighting scheme was *w* = 1/(*A* + *B*|*F<sub>o</sub>*| + *C*|*F<sub>o</sub>*|<sup>2</sup>) with *A* = 0.4999, *B* = 0.3020 and *C* = 0.0049. The fractional atomic coordinates are given in Table 1.

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

\* 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.

Table 1. Fractional atomic coordinates (×10<sup>4</sup>) with e.s.d.'s in parentheses

|        | <i>x</i>  | <i>y</i>   | <i>z</i>  |
|--------|-----------|------------|-----------|
| 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)  |

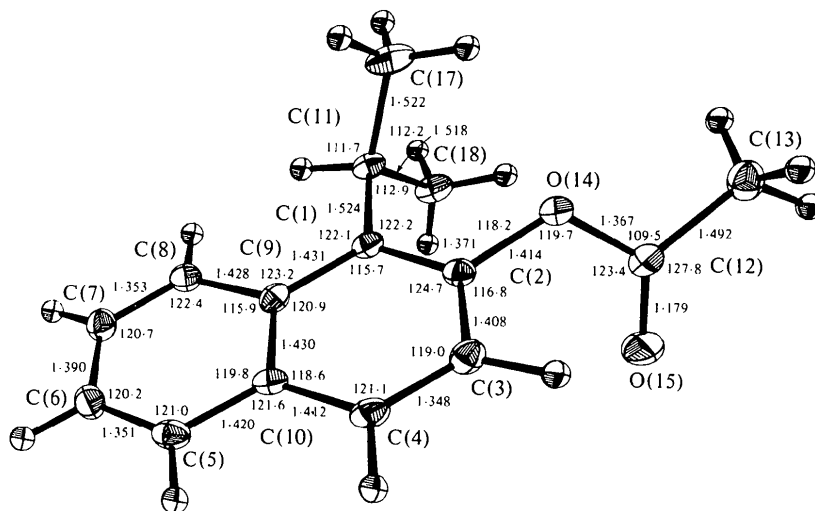


Fig. 1. A view of the molecule, showing bond lengths (Å) and bond angles (°).

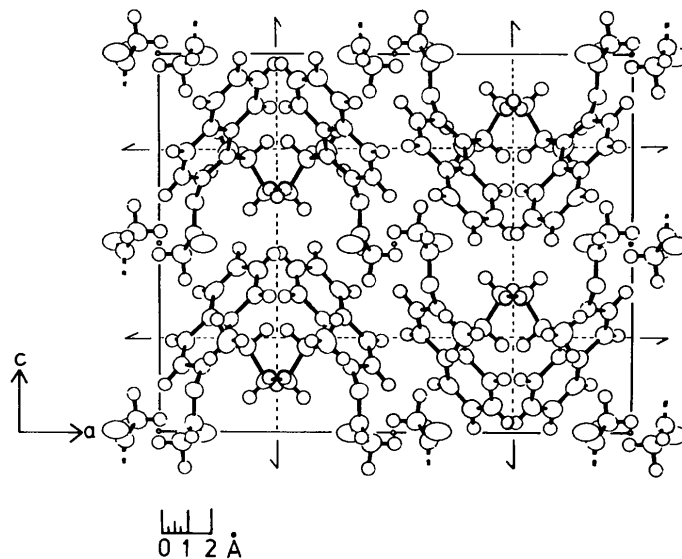


Fig. 2. The crystal packing.

increase in the C(1)–C(9)–C(8) angle consequent upon the replacement of a methyl (previous paper) by the isopropyl group (from 122.3 to 123.2°) and this angle would appear to be a useful indicator of *peri* strain. There is also an increase in the sum of the C(1)–C(9) and C(8)–C(9) lengths and a corresponding reduction in C(4)–C(10) and C(5)–C(10). The latter distortion also has the effect of moving H(8) and the 1-alkyl group away from each other; this has been noticed previously (Robert, Sherfinski, Marsh & Roberts, 1974). Apart from these effects there is

little distortion of the molecular geometry — a feature shared by 1,8-bis(dimethylamino)naphthalene (Einspahr, Robert, Marsh & Roberts, 1973).

The crystal packing is shown in Fig. 2.

#### References

- EINSPAHR, H., ROBERT, J. B., MARSH, R. E. & ROBERTS, J. D. (1973). *Acta Cryst.* B29, 1611–1617.  
ROBERT, J. B., SHERFINSKI, J. S., MARSH, R. E. & ROBERTS, J. D. (1974). *J. Org. Chem.* 39, 1152–1156.