N(2) is hydrogen bonded to O(3^{ii}) [(ii) = $\frac{1}{2}+x$, $-y-\frac{1}{2}$, $1-z$] with N···O and H···O lengths of 2·80 (2) and 2·16 (8) Å, respectively. The acetate group at C(17) in (II) shows a β-orientation. The C(13)—C(17)—O(20)—C(21) torsion angle is −160·9 (7)°, thus the acetate moiety is antiperiplanar with respect to the C(13)—C(17) bond and the O(22) atom is oriented to the α side of the molecule. The O(22) atom is synperiplanar to C(17) [C(17)—O(20)—C(21)—O(22) −1·1 (7)°]. The pseudo-torsion angles C(19)—C(10)···C(13)—C(18) are 2·0 (8)° in (I) and 0·0 (8)° in (II).

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Structure of Plumbagin*

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Abstract. $C_{11}H_8O_3$, $M_r = 188{\cdot}2$, monoclinic, $P2_1/a$, $a = 19{\cdot}067$ (3), $b = 7{\cdot}057$ (2), $c = 13{\cdot}370$ (3) Å, $\beta = 91{\cdot}17$ (2)°, $V = 1798{\cdot}6$ Å^3, $Z = 8$, $D_m = 1{\cdot}37$ (3), $D_x = 1{\cdot}390$ (1) Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}110$ mm^{-1}, $F(000) = 784$, $T = 298$ K, $R = 0{\cdot}066$ for 1426 reflections. There are two molecules in the asymmetric unit and they have slightly different geometry. The packing of the molecules is due to van der Waals forces and there are no intermolecular hydrogen bonds.

Introduction. Plumbagin is the active principle of chita, the root of plants under three distinct botanical classifications: (1) *Plumbago rosea*, (2) *P. zeylanica* and (3) *P. europoea*. Plumbagin is known for its chemotherapeutic properties. It is used in various prescriptions for dyspepsia, paralysis, rheumatism, coughs and leprosy (Roy & Dutt, 1928). The structure and synthesis of this compound has been carried out by Fieser & Dunn (1936) and its biosynthesis has been described by Durand & Zenk (1971).

Experimental. D_m by flotation, dark-yellow needles (from methanol) 0·4 × 0·5 × 0·4 mm, Enraf–Nonius CAD-4 diffractometer (at the Indian Institute of Technology, Madras), $\omega/2\theta$ scan technique, Mo $K\alpha$ radiation, cell parameters refined from 14 strong accurately centred reflections in the range $18 < 2\theta < 26°$, Lp correction, absorption ignored, 3220 unique reflections with $0 \le h \le 16$, $0 \le k \le 8$, $-16 \le l \le 16$ and with $2\theta \le 54°$, 1426 reflections with $|F_o| \ge 0{\cdot}5\sigma(|F_o|)$. Two standard reflections monitored every 100 reflections during data collection, intensity variation less than 5%. Structure solution using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), 290 reflections with $|E| \ge 1{\cdot}278$ for phase generation, most H atoms located from $\Delta\rho$ map. Full-matrix refinement on F (Gantzel, Sparks & Trueblood, 1961) with anisotropic temperature factors for non-H atoms and isotropic for H atoms, final $R = wR = 0{\cdot}066$, Cruickshank weighting scheme (Cruickshank, Bujosa, Lovell & Truter, 1961) with $w = 1/\sigma^2$ where $\sigma^2 = A + B|F_o| + C|F_o|^2$

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* 5-Hydroxy-2-methyl-1,4-naphthoquinone.

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Table 1. *Fractional positional parameters* (× 10^4) *of the non*-H *atoms with e.s.d.'s in parentheses and their equivalent isotropic thermal parameters*

The arithmetic mean of the principal axes of the thermal ellipsoid:

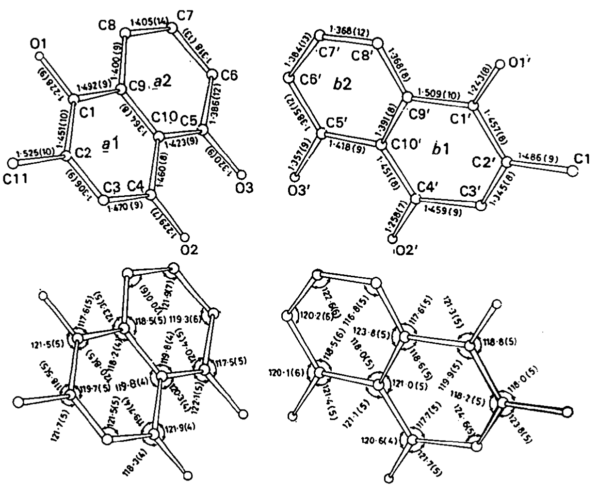
$$B_{eq}{}^* = \tfrac{4}{3}\textstyle\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}(Å^2)
C(1)	6000 (4)	3429 (10)	5506 (5)	6·1
C(2)	6242 (3)	3310 (9)	4486 (5)	5·5
C(3)	5800 (4)	2877 (10)	3763 (5)	5·5
C(4)	5072 (3)	2338 (9)	3966 (4)	4·7
C(5)	4125 (4)	1797 (10)	5202 (5)	6·1
C(6)	3889 (4)	1813 (10)	6175 (7)	7·4
C(7)	4321 (6)	2334 (11)	6907 (6)	7·9
C(8)	5015 (5)	2889 (12)	6730 (5)	7·1
C(9)	5267 (3)	2892 (6)	5754 (4)	3·9
C(10)	4820 (3)	2386 (8)	4990 (4)	4·3
C(11)	7009 (4)	3755 (12)	4286 (8)	8·8
O(1)	6395 (3)	3905 (9)	6198 (5)	9·4
O(2)	4688 (3)	1890 (7)	3256 (3)	7·0
O(3)	3681 (3)	1235 (9)	4492 (5)	8·7
C(1′)	8274 (4)	773 (9)	9660 (4)	5·3
C(2′)	8520 (3)	829 (8)	10698 (4)	4·3
C(3′)	8039 (3)	822 (9)	11420 (4)	5·1
C(4′)	7282 (3)	779 (7)	11239 (4)	4·6
C(5′)	6302 (4)	729 (10)	9969 (5)	5·9
C(6′)	6093 (4)	712 (11)	8971 (7)	7·6
C(7′)	6588 (5)	779 (10)	8229 (6)	7·3
C(8′)	7293 (4)	818 (9)	8434 (5)	6·0
C(9′)	7497 (4)	790 (9)	9420 (4)	4·7
C(10′)	7031 (3)	771 (8)	10207 (4)	4·1
C(11′)	9289 (3)	865 (10)	10899 (6)	6·5
O(1′)	8713 (3)	718 (9)	8987 (3)	8·4
O(2′)	6857 (2)	739 (8)	11946 (3)	7·1
O(3′)	5816 (3)	713 (8)	10695 (5)	8·3

* Hamilton (1959).

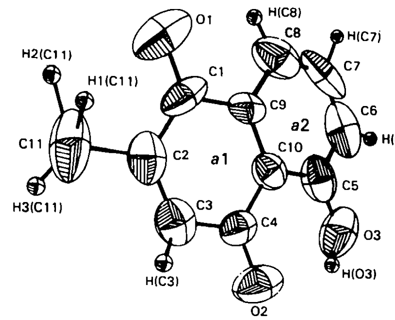
and $A = 8{\cdot}0$, $B = 1{\cdot}0$ and $C = 0{\cdot}01$; $(\Delta/\sigma)_{\max} = 0{\cdot}32$. The final difference synthesis showed no peaks either positive or negative exceeding 0·4 e Å^{-3}. The scattering factors for non-H atoms were from *International Tables for X-ray Crystallography* (1962) and for H atoms from Stewart, Davidson & Simpson (1965). All calculations were performed using an IBM 1130 at the University of Madras and an IBM 370 at the Indian Institute of Technology, Madras. Table 1* lists fractional positional parameters and equivalent isotropic thermal parameters.

Discussion. The bond lengths and angles of the two napthoquinone molecules A and B in the asymmetric unit are given in Fig. 1 and the corresponding *ORTEP* plots in Fig. 2. The bond lengths and angles in molecules A and B are almost normal. The geometries of molecules A and B are such that each of the molecules has an approximate pseudo centre of inversion on C(9)—C(10). Considering only the ring atoms of molecule A, this approximate pseudo centre of inversion is found to be at 0·506 (1), 0·261 (3), 0·534 (2) while it is found to be at 0·729 (2), 0·078 (2), 0·982 (1) for molecule B, both rather close to special positions. This aspect of the structure is reflected in the rather unusual distribution of the cumulative probability distribution of $N(Z)$ *versus* Z where Z is normalized intensity. In some cases, the distribution lies

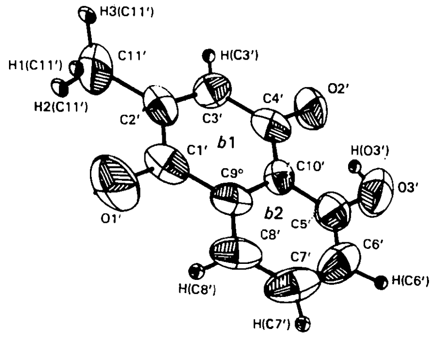


Molecule A Molecule B

Fig. 1. Perspective views of the molecules showing bond lengths (Å) and angles (°).



Molecule *A*



Molecule *B*

Fig. 2. *ORTEP* (Johnson, 1965) plots of the molecules with 50% probability thermal ellipsoids.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44190 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

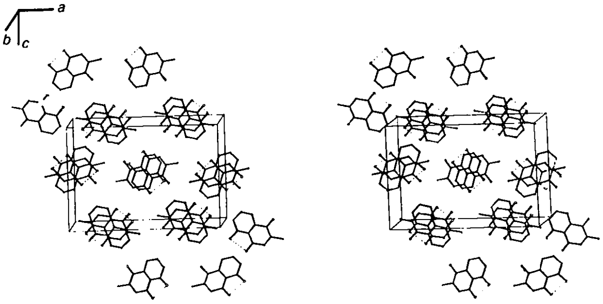

Fig. 3. Stereo packing diagram of the molecules.

between theoretical values for centrosymmetric and noncentrosymmetric distributions.

The planes of molecule *B* are stacked almost perpendicular to the *b* axis with a constant interplanar distance of 3·53 (2) Å. The naphthoquinone ring planes of *A* and *B* are at an angle of 17·2° to each other. The molecular layers of *A* are arranged at alternate distances of 3·52 (2) and 3·38 (2) Å.

A stereo plot of the molecule down the *b* axis with 10° rotation around both *x* and *z* axes using the molecular plotting program of Radhakrishnan (1982) is given in Fig. 3. In each of the molecules the hydrogen of the hydroxy group forms an intramolecular hydrogen bond with the carbonyl group. In molecule *A* the O(3)···O(2) distance is 2·599 (7) Å, H(O3)···O(2) is 1·87 (8) Å and the O(3)–H(O3)···O(2) angle is 130 (5)°. In molecular *B* O(3′)···O(2′) is 2·570 (7) Å, H(O3′)···O(2′) is 1·71 (15) Å and the O(3′)–H(O3′)···O(2′) angle is 161 (11)°. The crystal packing is stabilized by van der Waals forces.

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Structure of Ginkgolide A (BN52020) Monohydrate and Ginkgolide C (BN52022).Ethanol.1·5Hydrate, Isolated from *Ginkgo biloba* L.

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Abstract. Ginkgolide A monohydrate: 3-(1,1-dimethylethyl)hexahydro-4,7b-dihydroxy-8-methyl-9*H*-1,7a-(epoxymethano)-1*H*,6a*H*-cyclopenta[*c*]furo[2,3-*b*]-furo[3′,2′:3,4]cyclopenta[1,2-*d*]furan-5,9,12(4*H*)-trione monohydrate, $C_{20}H_{24}O_9.H_2O$, $M_r = 426·4$, orthorhombic, $P2_12_12_1$, $a = 8·9906$ (3), $b = 12·4256$ (10), $c = 17·8140$ (11) Å, $V = 1990·1$ (2) Å^3, $Z = 4$, $D_x = 1·423$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 8·2$ cm^{-1}, $T = 290$ K, $F(000) = 904$, final $R = 0·042$ for 1399 observed reflections. Ginkgolide C.ethanol.1·5hydrate: 3-(1,1-dimethylethyl)hexahydro-2,4,7b,11-tetrahydroxyl-8-methyl-9*H*-1,7a-(epoxymethano)-1*H*,6a*H*-cyclopenta[*c*]furo[2,3-*b*]furo[3′,2′:3,4]cyclopenta[1,2-*d*]-furan-5,9,12(4*H*)-trione.ethanol.1·5hydrate, $C_{20}H_{24}O_{11}.C_2H_6O.1·5H_2O$, $M_r = 513·5$, monoclinic, $P2_1$, $a = 12·9668$ (5), $b = 13·1218$ (6), $c = 15·3083$ (5) Å, $\beta = 112·95$ (3)°, $V = 2398·5$ (1) Å^3, $Z = 4$, $D_x = 1·422$ g cm^{-3}, μ(Cu $K\alpha$) = 9·1 cm^{-1}, $F(000) = 1092$,

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