C(31') with a distance between the hydrogen atoms of 2·3 Å and several intermolecular contacts (≤2·6 Å) corresponding to van der Waals forces. Four atoms from the O-benzyl group connected with C(3') participate in these contacts.

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Structure of 3,6,10,12-Tetramethylbenzofuro[2,3-b]benzofuran

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Abstract. $C_{18}H_{18}O_2$, $M_r = 266.3$, monoclinic, $P2_1/n$, $a = 9.459$ (2), $b = 13.220$ (2), $c = 11.712$ (2) Å, $\beta = 98.92$ (2)°, $V = 1446.8$ (5) Å^3, $D_m = 1.24$ (1), $D_x = 1.22$ g cm^{-3}, $Z = 4$, $\lambda(\text{Mo } K\alpha) = 0.7107$ Å, $\mu = 0.73$ cm^{-1}, $T = 293$ K, $F(000) = 568$, $R = 0.077$ and $wR = 0.077$ for 1250 reflections with $F \geq 3\sigma(F)$. The furan rings are in envelope conformation with an angle of 66·5 (3)° between them.

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† DCB contribution No. 745.

Introduction. The benzofuran ring system is prevalent in many natural products and some exhibit bactericidal activity (Gilchrist, 1985). The title compound was obtained as a by-product in the synthesis of pterocarpans (Ramakanth, 1984). The present paper reports the X-ray structure of the compound in the crystal.

Experimental. Colourless needle-shaped single crystals by slow evaporation of acetone, D_m by flotation, $0.35 \times 0.30 \times 0.25$ mm, monoclinic $P2_1/n$, three-

Table 1. *Positional parameters and equivalent iso-tropic temperature factors of non-hydrogen atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

|	x	y	z	B_{eq}(Å²)
O1	0·8110 (4)	0·2371 (3)	0·1668 (4)	4·5 (2)
O2	0·6133 (4)	0·1553 (4)	0·2165 (3)	4·4 (2)
C1	0·6290 (7)	0·5579 (5)	−0·1449 (6)	5·5 (4)
C2	0·6784 (6)	0·4737 (4)	−0·0596 (5)	3·6 (2)
C3	0·6170 (6)	0·3771 (4)	−0·0694 (5)	3·7 (2)
C4	0·6639 (5)	0·3000 (4)	0·0075 (4)	2·9 (2)
C5	0·7718 (6)	0·3226 (4)	0·0981 (5)	3·4 (2)
C6	0·8376 (7)	0·4147 (6)	0·1110 (6)	5·1 (3)
C7	0·7886 (7)	0·4902 (5)	0·0319 (6)	4·7 (3)
C8	0·6192 (6)	0·1913 (4)	0·0156 (5)	3·3 (2)
C9	0·7110 (6)	0·1577 (4)	0·1319 (5)	3·4 (2)
C10	0·4682 (6)	0·1814 (4)	0·0424 (4)	3·0 (2)
C11	0·3364 (5)	0·1936 (4)	−0·0266 (4)	2·8 (2)
C12	0·2105 (6)	0·1843 (4)	0·0216 (5)	3·8 (3)
C13	0·2232 (6)	0·1634 (4)	0·1388 (5)	3·8 (3)
C14	0·3541 (6)	0·1521 (5)	0·2113 (5)	4·1 (3)
C15	0·4753 (6)	0·1615 (4)	0·1589 (5)	3·4 (2)
C16	0·0674 (7)	0·1968 (6)	−0·0499 (7)	4·0 (4)
C17	0·6414 (6)	0·1303 (5)	−0·0934 (5)	4·4 (3)
C18	0·7895 (7)	0·0575 (5)	0·1387 (6)	5·0 (3)
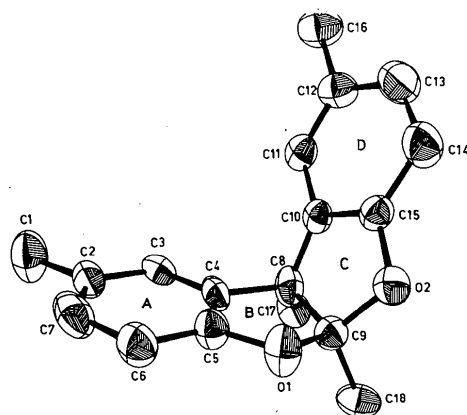
Fig. 1. *ORTEP* plot showing the thermal ellipsoids drawn at 50% probability level for the non-hydrogen atoms.

dimensional intensity data from an Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, cell parameters refined with 24 strong reflections in the range $16 \le 2\theta \le 32°$, 2124 unique reflections collected in the limit $0 \le 2\theta \le 47°$, $\theta/2\theta$ scan mode, 1250 reflections with $F \ge 3\sigma(F)$ considered as observed reflections, data corrected for Lorentz and polarization effects, no absorption cor-rection ($\mu r < 1$), structure solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), structure solution revealed all the non-hydrogen atoms, many of the hydrogens were fixed geometrically, isotropic refinement of non-hydrogens using *SHELX*76 (Shel-drick, 1976) and later anisotropic refinement of non-hydrogens using *LALS* (Gantzel, Sparks & True-blood, 1961), Hughes (1941) weighting scheme with

$(F_o)_{min} = 3·6$, hydrogens included only in structure-factor calculation and not in refinement with assigned temperature factors of non-hydrogens to which they are attached. Final $R = 0·077$ and $wR = 0·077$. The rather high R factor is due to the poor
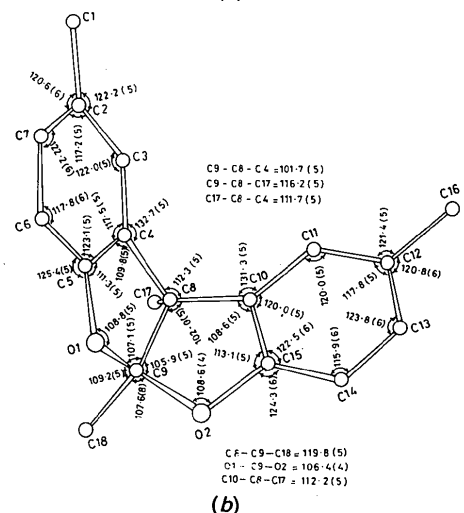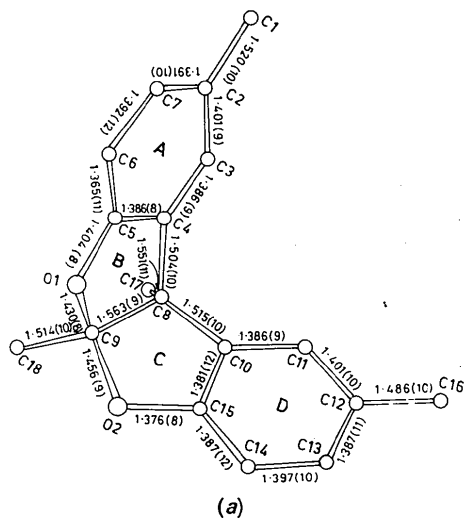

(a)

(b)

Fig. 2. (a) Bond lengths (Å) involving non-hydrogen atoms. (b) Bond angles (°) involving non-hydrogen atoms.
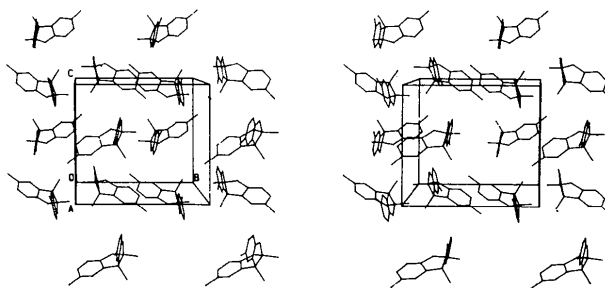

Fig. 3. Stereoview of the packing of the molecules in the unit cell.

quality of data and many hydrogen positions, fixed geometrically, were not refined. The final (shift/e.s.d)$_{ave}$ = 0·033 and (shift/e.s.d.)$_{max}$ = 0·097. A final difference Fourier showed no peaks $\geq 0\cdot3\,e\,\text{Å}^{-3}$. Scattering factors for non-hydrogen atoms were taken from *International Tables for X-ray Crystallography* (1968) and for hydrogens from Stewart, Davidson & Simpson (1965).

Discussion. The final fractional coordinates with equivalent temperature factors of non-hydrogens are given in Table 1. Thermal ellipsoids drawn at 50% probability level for non-hydrogens using *ORTEP* (Johnson, 1965) are shown in Fig. 1.*

The bond lengths and angles involving non-hydrogen atoms are shown in Figs. 2(*a*) and 2(*b*) respectively. The e.s.d.'s in bond lengths are 0·010 Å and in bond angles 0·5°. The bond lengths and angles in the two benzofuran ring systems are comparable with those in similar structures.

The torsion angles around the two furan rings *B* and *C* show that they are in envelope conformation with $C_s = 1\cdot39$ and 0·80 respectively (Duax, Weeks & Rohrer, 1976). In both cases, the envelope atom C9 is out of the plane of the other four atoms in the furan rings *B* and *C* by 0·2 and 0·16 Å respectively. The two benzofuran moieties are planar. The angle between the planes of the two furan rings is 66·5°. This compares with 64·8° in a dihydrobenzofuro-[3,2-*b*]benzofuran derivative (Wong & Jurd, 1984).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52300 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The two methyl carbons C1 and C16 are in the plane of the benzene rings to which they are attached. The torsion angle C17—C8—C9—C18, −13·9 (1)°, shows that C17 and C18 are *cis* with respect to the C8—C9 bond.

A stereoview of the unit-cell packing (Motherwell, 1978) is shown in Fig. 3. The molecules are stabilized in the unit cell by van der Waals interactions.

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Structure of the Thromboxane Receptor Antagonist EP 092

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Abstract. 7-{3-[1-(4-Phenylthiosemicarbazono)ethyl]-bicyclo[2.2.1]hept-2-yl}-5-heptenoic acid, $C_{23}H_{31}N_3O_2S$, $M_r = 413\cdot7$, monoclinic, $P2_1/a$, $a = 12\cdot9650$ (7), $b = 11\cdot2081$ (6), $c = 16\cdot8941$ (12) Å, $\beta = 110\cdot452$ (5)°, $V = 2300\cdot2$ Å^3, $Z = 4$, $D_x = 1\cdot194$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71073$ Å, $\mu = 1\cdot55$ cm^{-1}, $F(000) = 888$, $T = 298$ K.