The atoms deviate by a maximum of 0·022 Å from the plane of the whole molecule; thus it is planar within experimental error to a significance level of about 0·5 according to a χ^2 test. (The isotropic e.s.d.'s for the atomic positions are 0·012–0·016 Å.) The benzene rings *A* and *C* are planar to within ±0·003 and ±0·012 Å, respectively, and the furan rings *B* and *D* are planar to within ±0·009 and ±0·007 Å, respectively.

The molecules are stacked along the short *a* axis, as indicated by the packing diagram in Fig. 2. All intermolecular contacts correspond to normal van der Waals distances. The distance of closest approach between adjacent molecules is 3·74 (1) Å. In spite of the non-interacting distances, the packing is very dense, as reflected in the high D_x of 1·664 (1) Mg m^{-3}. The packing coefficient, *i.e.* the ratio between the volume occupied by the four molecules and the cell volume, is 0·75.

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Quinone Oligomerization. V.* Structure of Benzo[1,2-*b*:6,5-*b'*]bis[1]benzofuran, $C_{18}H_{10}O_2$

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Abstract. $M_r = 258{\cdot}35$, monoclinic, $P2_1/c$, $a = 4{\cdot}720\,(1)$, $b = 21{\cdot}274\,(3)$, $c = 12{\cdot}360\,(2)$ Å, $\beta = 96{\cdot}23\,(2)°$, $Z = 4$, $V = 1233{\cdot}8\,(6)$ Å^3, $D_x = 1{\cdot}391\,(1)$ Mg m^{-3}, $\mu(\text{Cu }K\alpha) = 0{\cdot}73$ mm^{-1}, $F(000) = 536$. The final *R* value is 0·040 for 1082 data collected at ambient temperature using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) and with $I_{\text{net}} \geq 4\sigma(I_{\text{net}})$. The molecule is significantly non-planar with an angle of 4·1 (3)° between the outer benzene rings.

Introduction. In our project on condensation products of quinones (Berg, Erdtman, Högberg, Karlsson, Pilotti & Söderholm, 1977), we have earlier reported the structures of a dimer and a trimer (Berg, Karlsson, Pilotti & Söderholm, 1978, 1980), an open tetramer (Karlsson, Pilotti & Söderholm, 1980) and a cyclic tetramer (Karlsson, Pilotti & Söderholm, 1983). These compounds consist of dibenzofuran elements which in the trimer and tetramers are connected in a cyclic way giving cyclic or partly cyclic or helical structures. The open tetramer shows considerable steric overcrowding. In the present study we have determined the structure of an oligomer in which the dibenzofuran elements are connected in a linear way, and hence are free from close intramolecular contacts.

Experimental. Needle-shaped crystal, ~0·45 × 0·08 × 0·06 mm; lattice parameters from least-squares treatment of the angular coordinates of 25 well centered reflexions, Philips PW1100 diffractometer, graphite

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* Part IV: Karlsson, Pilotti & Söderholm (1983).

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monochromator; $2\theta_{\max} = 140°$, θ–2θ scan technique, three standard reflexions measured hourly; 2362 measured reflexions ($0 \le h \le 5$, $0 \le k \le 25$, $|l| \le 15$), 1082 unique reflexions with $I_{\rm net} \ge 4\sigma(I_{\rm net})$; correction for Lorentz–polarization but not absorption. Direct methods [*MULTAN* (Germain, Main & Woolfson, 1971)] using the 200 highest E values in 900 triple-phase relationships; all non-hydrogen atoms from an E map based on the phase set having the highest figure of merit; full-matrix least-squares refinement based on $|F|$ [*LALS* (Gantzel, Sparks & Trueblood, 1966)], all H atoms from a ΔF map; subsequent least-squares refinements (anisotropic thermal parameters for the non-hydrogen atoms and fixed isotropic temperature factors of 3·5 Å^2 for H atoms) gave a final R of 0·040, identical to wR using the scheme of Hughes (1941) and an $|F_{o,\min}|$ of 3·5; $S = 0·040$, $\Delta/\sigma \le 0·05$, $\Delta\rho$ in final difference map −0·2–0·2 e Å^{-3}; scattering factors for non-hydrogen atoms from *International Tables for X-ray Crystallography* (1962), and for H from Stewart, Davidson & Simpson (1965).

Discussion. The final positional parameters are listed in Table 1 for the non-hydrogen atoms together with calculated $B_{\rm eq}$ values.* The molecular geometry is shown in Fig. 1, which also gives the numbering system used and the interatomic bond distances for the non-hydrogen atoms. Bond angles are given in Table 2.

Table 1. *Positional parameters with e.s.d.'s in parentheses*

Equivalent isotropic thermal parameters (Å^2) are given for the non-hydrogen atoms.

	x	y	z	$B_{\rm eq}$
C(1)	0·8159 (8)	0·9833 (2)	0·6348 (4)	5·36 (11)
C(2)	0·9692 (8)	1·0231 (2)	0·7066 (4)	6·10 (13)
C(3)	0·9469 (8)	1·0208 (2)	0·8166 (4)	6·14 (13)
C(4)	0·7661 (9)	0·9788 (2)	0·8603 (4)	6·05 (12)
C(4a)	0·6151 (7)	0·9395 (2)	0·7872 (3)	4·58 (9)
O(5)	0·4244 (5)	0·8936 (1)	0·8155 (2)	5·00 (7)
C(5a)	0·3283 (6)	0·8658 (2)	0·7186 (3)	3·94 (8)
C(5b)	0·1345 (6)	0·8171 (2)	0·7014 (3)	3·79 (8)
O(6)	−0·0084 (5)	0·7875 (1)	0·7792 (2)	4·66 (6)
C(6a)	−0·1716 (6)	0·7416 (2)	0·7213 (3)	3·98 (8)
C(7)	−0·3534 (7)	0·7012 (2)	0·7671 (3)	4·80 (10)
C(8)	−0·4967 (8)	0·6586 (2)	0·6980 (3)	5·06 (10)
C(9)	−0·4617 (8)	0·6565 (2)	0·5880 (3)	4·94 (10)
C(10)	−0·2789 (7)	0·6976 (2)	0·5432 (3)	4·50 (9)
C(10a)	−0·1338 (6)	0·7417 (2)	0·6112 (3)	3·83 (8)
C(10b)	0·0679 (6)	0·7922 (2)	0·5980 (3)	3·91 (8)
C(11)	0·1905 (7)	0·8175 (2)	0·5086 (3)	4·43 (9)
C(12)	0·3766 (7)	0·8672 (2)	0·5254 (3)	4·65 (9)
C(12a)	0·4474 (6)	0·8909 (2)	0·6294 (3)	3·90 (8)
C(12b)	0·6350 (6)	0·9399 (2)	0·6763 (3)	4·17 (9)

Table 2. *Bond angles* (°) *involving the non-hydrogen atoms* (*e.s.d.'s* 0·2–0·4°, *mean* 0·3°) *and pertinent torsion angles* (°) *for the perimeter of the molecule* (*e.s.d.'s* 0·4–0·7°)

C(2)–C(1)–C(12b)	118·1	C(6a)–C(7)–C(8)	116·3
C(1)–C(2)–C(3)	121·1	C(7)–C(8)–C(9)	121·8
C(2)–C(3)–C(4)	121·6	C(8)–C(9)–C(10)	121·1
C(3)–C(4)–C(4a)	115·6	C(9)–C(10)–C(10a)	118·2
C(4)–C(4a)–O(5)	124·3	C(6a)–C(10a)–C(10)	118·9
C(4)–C(4a)–C(12b)	124·1	C(6a)–C(10a)–C(10b)	105·4
O(5)–C(4a)–C(12b)	111·6	C(10)–C(10a)–C(10b)	135·7
C(4a)–O(5)–C(5a)	104·1	C(5b)–C(10b)–C(10a)	105·3
O(5)–C(5a)–C(5b)	127·5	C(5b)–C(10b)–C(11)	120·4
O(5)–C(5a)–C(12a)	113·8	C(10a)–C(10b)–C(11)	134·3
C(5b)–C(5a)–C(12a)	118·8	C(10b)–C(11)–C(12)	119·0
C(5a)–C(5b)–O(6)	126·7	C(11)–C(12)–C(12a)	120·3
C(5a)–C(5b)–C(10b)	120·4	C(5a)–C(12a)–C(12)	121·1
O(6)–C(5b)–C(10b)	112·8	C(5a)–C(12a)–C(12b)	103·9
C(5b)–O(6)–C(6a)	104·3	C(12)–C(12a)–C(12b)	135·1
O(6)–C(6a)–C(7)	124·1	C(1)–C(12b)–C(4a)	118·7
O(6)–C(6a)–C(10a)	112·2	C(1)–C(12b)–C(12a)	134·6
C(7)–C(6a)–C(10a)	123·6	C(4a)–C(12b)–C(12a)	106·7

C(3)–C(4)–C(4a)–O(5)	179·4
C(4)–C(4a)–O(5)–C(5a)	−179·3
C(4a)–O(5)–C(5a)–C(5b)	180·0
O(5)–C(5a)–C(5b)–O(6)	1·9
C(5a)–C(5b)–O(6)–C(6a)	−178·9
C(5b)–O(6)–C(6a)–C(7)	−178·8
O(6)–C(6a)–C(7)–C(8)	−179·6
C(9)–C(10)–C(10a)–C(10b)	−179·0
C(10)–C(10a)–C(10b)–C(11)	2·1
C(10a)–C(10b)–C(11)–C(12)	179·2
C(10b)–C(11)–C(12)–C(12a)	1·6
C(11)–C(12)–C(12a)–C(12b)	178·0
C(12)–C(12a)–C(12b)–C(1)	1·0
C(12a)–C(12b)–C(1)–C(2)	−178·8

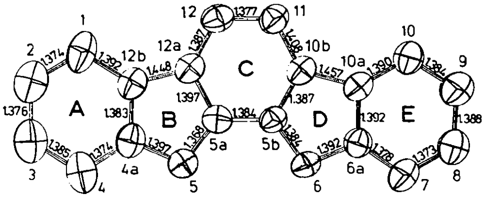

Fig. 1. *ORTEP* drawing (Johnson, 1965) of the molecule showing the bond distances (Å) and the numbering scheme. E.s.d.'s are 0·003–0·007 Å (mean 0·005 Å). O atoms are shaded.

The five rings form a conjugated system. The bond lengths within the six-membered rings are in the range 1·373 (5) to 1·408 (4) Å, whereas the C(sp^2)–C(sp^2) single bonds in the five-membered rings are 1·448 (4) and 1·457 (4) Å. These values are in accordance with those of other compounds containing dibenzofuran elements, *e.g.* leucothelephoric acid hexamethyl ether (Silverton, 1973), gnidicoumarin (Shen & Bryan, 1975), ruscodibenzofuran (El Sohly *et al.*, 1977), penioflavin diacetate (Hiltunen, Niinistö, Pakkanen & Pakkanen, 1978), 2,3,7,8-tetrachlorodibenzofuran (Hubbard, Mighell & Pomerantz, 1978), 2-(4-dibenzofuryloxy)-2-methylpropionic acid (Wägner & Malmros, 1979) as well as for those structures reported within this project (Berg *et al.*, 1978, 1980; Karlsson *et al.*, 1983). For the

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* Lists of anisotropic temperature factors, coordinates of the H atoms and structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38619 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

dibenzofuran molecule itself the $C(sp^2)$—$C(sp^2)$ single bond in the five-membered ring is 1·480 (6) Å (Banerjee, 1973, 1974) and 1·481 (3) Å (Dideberg, Dupont & André, 1972), *i.e.* significantly longer than those observed by us and others. In the dibenzofuran trimer (part III of this series), where severe overcrowding is observed, bond lengths in the six-membered rings along the inner periphery of the molecule are as long as 1·445–1·455 Å.

The C—H distances vary in the range 0·87 to 1·01 Å, e.s.d. 0·03 Å, mean value 0·94 Å, and are hence quite normal. Intramolecular angles show no significant deviations from expected values.

The maximum deviation from planarity in the individual rings is found for ring *C* (0·014 Å). The corresponding value for ring *E* is 0·010 Å, for the other rings <0·006 Å, and for the molecule as a whole 0·073 Å. The isotropic e.s.d.'s for the atomic positions are 0·002–0·004 Å. The molecule is thus significantly non-planar. The five-membered rings (*B* and *D*) are planar to a significance level of about 0·5 according to a χ^2 test.

Of the six-membered rings, ring *A* is roughly planar, whereas rings *C* and *E* are not strictly planar within experimental errors. The angle between the outer rings, *A* and *E*, is 4·1 (3)° and that between *B* and *D* is 2·5 (2)°. Selected torsion angles along the perimeter of the molecule are given in Table 2. The non-planarity of the system is probably influenced by dibenzofuran itself appearing to have a slight boat shape, as observed in other X-ray determinations of substituted dibenzofurans (Berg *et al.*, 1978; Wägner & Malmros, 1979). However, Hiltunen *et al.* (1978) reported that the central dibenzofuran fragment of penioflavin diacetate is planar.

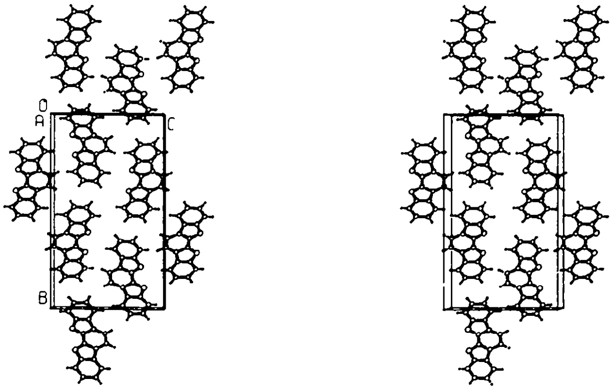

Fig. 2. Stereoscopic view [*PLUTO*78 (Motherwell & Clegg, 1978)] of the molecular packing.

The arrangement of molecules in the unit cell is shown in Fig. 2. The shortest intermolecular distances are found between equivalent molecules along the short *a* axis. However, all these are longer than 3·5 Å.

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