form a spiral. The angles between the least-squares planes of the attached phenyl ring [C(4), C(5), C(6), C(7), C(8), C(9)] and those defined by C(9), C(1), O, C(2) and C(1), C(2), C(3), C(10) are 3·2 and 8·0° respectively. The planar phenyl rings are twisted with respect to each other at an angle of 15·3°. This value is copmparable with the 11·4° for chalcone (Rabinovich, 1970) and differs markedly from the 52·9° for 2-benzylidene-1-tetralone (Kałuski *et al.*, 1978).

The arrangement of molecules in the unit cell (projection *xOz*) is shown in Fig. 2. The closest intermolecular contacts are: $O(x,y,z)\cdots C(8)(-x,-y,-z) = 3{\cdot}410\,(6)$ Å and $O(x,y,z)\cdots C(3)(x, y, z-1) = 3{\cdot}482\,(5)$ Å. All other interactions are of van der Waals type.

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Structure of 2,11-Dimethoxybenzo[1,2-*b*;4,3-*b*′]bis(benzofuran)*

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Abstract. $C_{20}H_{14}O_4$, orthorhombic, $P2_12_12_1$, $a = 18{\cdot}100\,(3)$, $b = 15{\cdot}026\,(2)$, $c = 5{\cdot}509\,(2)$ Å, $Z = 4$, $V = 1498$ Å^3, $D_x = 1{\cdot}41$ Mg m^{-3}, $\mu(\mathrm{Cu}\,K\alpha) = 82$ mm^{-1}. The final *R* value is 0·035 from 1158 data points for which $I_{\rm net} \geq 4\sigma(I_{\rm net})$. The molecule is not quite planar; the angles between adjacent ring planes vary from 0·8 to 2·2°. The distortion from a planar configuration is due to intramolecular overcrowding between H atoms.

Introduction. The crystal structure analysis of the title compound is part of a program of studies of quinone condensation products. The structure of the dimer 2,8-dimethoxydibenzofuran has been reported (part I). We now describe the molecular and crystal structure of the trimer 2,11-dimethoxybenzo[1,2-*b*;4,3-*b*′]bis(benzofuran).

X-ray intensities were collected on an automatic Philips PW 1100 diffractometer with monochromated Cu $K\alpha$ radiation, using the $\theta/2\theta$ scan technique. Of the 1345 reflexions collected ($\theta \leq 60°$), 1138 having $I_{\rm net} \leq 4\sigma(I_{\rm net})$ were considered observed. Lorentz and polarization corrections were applied but the intensities were not corrected for absorption effects [$\mu(\mathrm{Cu}\,K\alpha) = 82$ mm^{-1}; crystal dimensions $0{\cdot}50 \times 0{\cdot}10 \times 0{\cdot}075$ mm]. The unit-cell parameters were obtained from a least-squares fit of the angular coordinates for 25 reflexions measured on the diffractometer. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). The most probable *E* map showed 19 out of the 24 non-hydrogen atoms. The remaining atoms, including the hydrogens, were obtained from successive difference Fourier maps. The structure was refined by standard full-matrix least-squares methods, using unit weights, to an *R* value of 0·035. The H atoms were included in the refinement with fixed isotropic thermal parameters, equal to those of their parent atoms. Scattering factors for C and O were taken from Cromer & Mann (1968) and for H from

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* Quinone Oligomerization. II. Part I: Berg, Karlsson, Pilotti & Söderholm (1978).

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Stewart, Davidson & Simpson (1965). Final atomic coordinates are given in Table 1.*

Discussion. Fig. 1 is an *ORTEP* (Johnson, 1965) drawing of the molecule. Bond lengths and angles and the atom numbering are given in Fig. 2. Standard deviations are estimated to be of the order of 0·006 Å and 0·4°, respectively, for the non-hydrogen atoms. The average C—H distance is 1·02 Å.

The five fused rings form a conjugated system with C$\overset{...}{-}$C bond lengths ranging from 1·367 to 1·409 Å and C$\overset{...}{-}$O from 1·380 to 1·386 Å. These results conform with studies on the dimer mentioned above, 2-(4-dibenzofuranyloxy)-2-methylpropionic acid (Malmros & Wägner, 1980) and the related compounds dibenzothiophene–trinitrobenzene (Bechtel, Chasseau, Gaultier & Hauw, 1977) and 3-amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole (Itai & Iitaka, 1978).

The C—C—O angles around C(2) and C(11) are enlarged on the side of the methyl groups. This enlargement is probably due to steric interaction between ring and methyl hydrogens: H(C3)···H1(C14) = 2·18, H(C3)···H2(C14) = 2·26, H(C12)···H1(C16) = 2·36 and H(C12)···H2(C16) =

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

Values are $\times 10^4$ for the non-hydrogen atoms and $\times 10^3$ for the hydrogens.

	x	*y*	*z*
C(1)	4386 (2)	290 (2)	12991 (7)
C(2)	4148 (2)	−221 (2)	14940 (8)
C(3)	4645 (2)	−693 (2)	16387 (8)
C(4)	5394 (2)	−665 (2)	15871 (8)
C(4a)	5621 (2)	−164 (2)	13938 (7)
O(5)	6346 (1)	−74 (1)	13201 (5)
C(5a)	6327 (2)	492 (2)	11230 (8)
C(6)	6953 (2)	736 (3)	9923 (10)
C(7)	6872 (2)	1305 (3)	7975 (10)
C(7a)	6164 (2)	1589 (2)	7452 (9)
O(8)	6012 (1)	2136 (1)	5488 (5)
C(8a)	5254 (2)	2241 (2)	5498 (8)
C(9)	4864 (3)	2732 (3)	3806 (8)
C(10)	4111 (2)	2753 (3)	4033 (9)
C(11)	3750 (2)	2316 (2)	5935 (8)
C(12)	4145 (2)	1834 (2)	7670 (8)
C(12a)	4918 (2)	1791 (2)	7416 (8)
C(12b)	5523 (2)	1354 (2)	8701 (7)
C(12c)	5604 (2)	772 (2)	10689 (7)
C(12d)	5137 (2)	327 (2)	12465 (8)
O(13)	3395 (1)	−204 (2)	15361 (6)
C(14)	3127 (3)	−690 (4)	17418 (11)
O(15)	3003 (1)	2404 (2)	5937 (7)
C(16)	2594 (3)	1956 (4)	7772 (13)
H(C1)	401 (1)	61 (2)	1220 (7)
H(C3)	444 (2)	−107 (2)	1780 (7)
H(C4)	579 (1)	−99 (2)	1680 (7)
H(C6)	741 (2)	50 (2)	1039 (9)
H(C7)	732 (2)	144 (2)	696 (8)
H(C9)	513 (2)	302 (2)	247 (9)
H(C10)	375 (2)	312 (2)	293 (8)
H(C12)	387 (2)	150 (2)	890 (7)
H1(C14)	337 (2)	−59 (3)	1901 (9)
H2(C14)	257 (2)	−54 (2)	1768 (9)
H3(C14)	323 (2)	−141 (2)	1745 (8)
H1(C16)	268 (2)	121 (2)	730 (9)
H2(C16)	210 (2)	210 (2)	758 (9)
H3(C16)	272 (2)	225 (3)	956 (9)

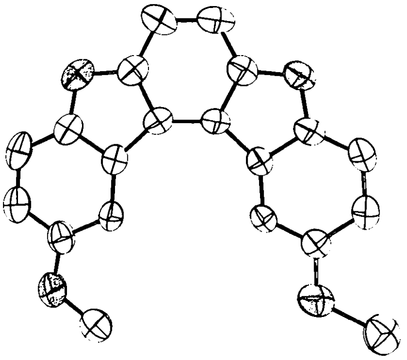

Fig. 1. An *ORTEP* drawing of the molecule.

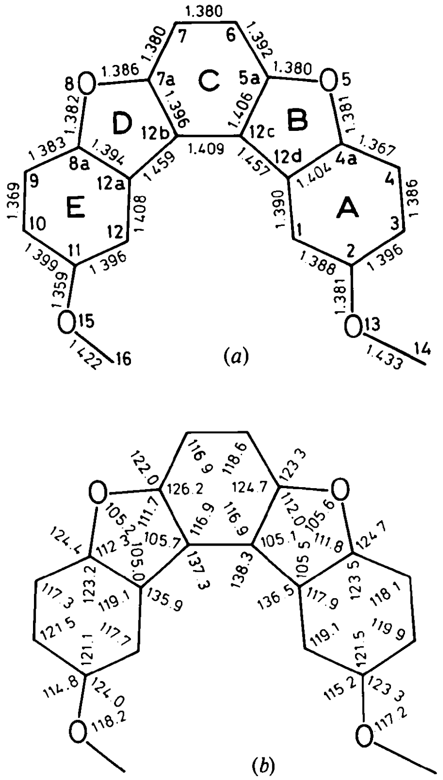

Fig. 2. (*a*) Bond distances (Å) and numbering scheme. (*b*) Bond angles (°).

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[*] Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35064 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Torsion angles (°) with e.s.d.'s in parentheses for the perimeter of the molecule*

C(12d)–C(1)–C(2)–C(3)	0·4 (7)	C(5a)–C(6)–C(7)–C(7a)	−0·4 (8)	C(10)–C(11)–C(12)–C(12a)	−1·0 (7)
C(1)–C(2)–C(3)–C(4)	−0·8 (8)	C(6)–C(7)–C(7a)–O(8)	−177·7 (8)	C(11)–C(12)–C(12a)–C(12b)	−177·4 (8)
C(2)–C(3)–C(4)–C(4a)	0·3 (7)	C(7)–C(7a)–O(8)–C(8a)	177·4 (6)	C(12)–C(12a)–C(12b)–C(12c)	2·1 (9)
C(3)–C(4)–C(4a)–O(5)	−180·0 (7)	C(7a)–O(8)–C(8a)–C(9)	−179·0 (6)	C(12a)–C(12b)–C(12c)–C(12d)	−1·0 (9)
C(4)–C(4a)–O(5)–C(5a)	−179·2 (6)	O(8)–C(8a)–C(9)–C(10)	178·4 (8)	C(12b)–C(12c)–C(12d)–C(1)	−0·9 (9)
C(4a)–O(5)–C(5a)–C(6)	−178·5 (6)	C(8a)–C(9)–C(10)–C(11)	1·7 (8)	C(12c)–C(12d)–C(1)–C(2)	−178·8 (8)
O(5)–C(5a)–C(6)–C(7)	180·0 (8)	C(9)–C(10)–C(11)–C(12)	−0·5 (8)		

2·40 Å. The molecule is not quite planar which is probably an effect of overcrowding between the H atoms attached to C(1) and C(12). In a coplanar, undistorted molecule the distance between H(C1) and H(C12) would be approximately 1·6 Å. These atoms are hence bent away from each other to achieve a clearance of 2·27 Å. The bending of the compound is distributed over the rings so as not to cause severe puckering or angle distortion in any individual ring. The deviations from planarity are within ±0·07 Å. Isotropic e.s.d.'s are of the order of 0·005 Å for the atoms. Values of the deviations from least-squares planes calculated for the individual rings and for the whole molecule are shown in Fig. 3. The interplanar angles between the consecutive rings *A*, *B*, *C*, *D* and *E* are 0·8, 1·1, 2·1, and 1·4°, respectively. Torsion angles (Table 2) around the inner core of the molecule, *i.e.* the bonds C(1)–C(12d), C(12d)–C(12c), C(12c)–C(12b), C(12b)–C(12a) and C(12a)–C(12), are −178·8, −0·9, −1·0, 2·1 and −177·4°, respectively. The fact that the dimer (part I) is also non-planar probably contributes to the non-planarity of the trimer.

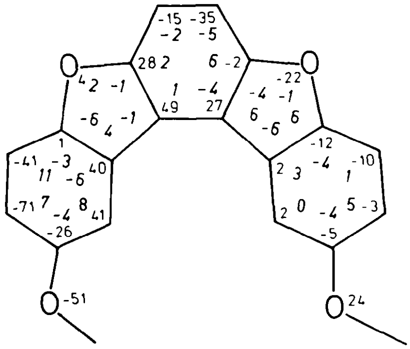

Fig. 3. Deviations from least-squares planes (Å, ×10³) for the individual rings (inner values) and for the whole molecule.

The methoxy groups are oriented away from each other (Fig. 1) in order to avoid close intramolecular contacts. There are no intermolecular distances shorter than the sum of the relevant van der Waals radii; the shortest non-hydrogen distance is C(8a)···C(12d) = 3·33 Å.

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