atom-labelling scheme in this paper is that recommended by the IUPAC–IUB Commission on Biochemical Nomenclature (1970)]. The distances are quite similar to the values found in both the α and β forms of L-Glu (except for C—H, N—H and O—H because the structures of L-Glu were solved on the basis of neutron diffraction). As can be seen in Fig. 1 the α-carboxyl group is ionized and the proton is transferred to the amino group. The γ-carboxyl group is in the un-ionized form. Ionized and protonated carboxyl groups are quite planar [maximum atomic deviation 0·002 (2) Å].* The $C—C^{\alpha}$ bond length to the ionized α-carboxyl group (1·528 Å) is significantly longer than the $C^{\gamma}—C^{\delta}$ bond to the protonated γ-carboxyl group (1·502 Å). This trend also occurs in both modifications of L-Glu and in the structures of DL-aspartic acid, DL-Asp (Rao, 1973), and L-aspartic acid, L-Asp (Derissen, Endeman & Peerdeman, 1968). The average difference in bond length between $C—C^{\alpha}$ to the ionized carboxyl group and $C^{\beta}—C^{\gamma}$ (for DL-Asp and L-Asp) or $C^{\gamma}—C^{\delta}$ (for DL-Glu and the α and β forms of L-Glu) to the protonated carboxyl group for all these structures is 0·030 (3) Å.

The conformation of glutamic acid in DL-Glu.H_2O crystals is different from those in the α and β forms of L-Glu (Table 2*c*). The α-amino part of the molecule is nearly planar. The deviation of the N atom from the $C^{\alpha}CO(1)O(2)$ plane is 0·050 (2) Å and the O(1)—C—C^{α}—N torsion angle (ψ^1) is—2·2°;C^{δ} is *gauche* to C and N. This implies that C^{δ} is *trans* to C^{α}, being the only possible conformation. The side chain is almost planar, and coplanar with the γ-carboxyl group.

The structure is strongly hydrogen-bonded.* Each molecule of glutamic acid is bound to adjacent molecules of glutamic acid and water through nine H-bonds. O(1), $O^{\varepsilon}(1)$ and $O^{\varepsilon}(2)$ each accepts one H bond and O(2) accepts two H-bonds. The donors are $O^{\varepsilon}(2)$ and N, involved in one and three H-bonds respectively. The water molecule is the acceptor of one and the donor of two weak H-bonds. $O^{\varepsilon}(2)—H^{\varepsilon}(2)\cdots O(2^{iv})$ of length 2·574 Å is stronger than the others. This intermolecular H-bond is similar to the bonds found in the α and β forms of L-Glu, more extensively described by Lehmann & Nunes (1980), L-Asp and DL-Asp.

This work was supported by the Polish Academy of Science.

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* See deposition footnote.

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Quinone Oligomerization. IV.* Structure of Tetraphenyleno[1,16-*bcd*:4,5-*b'c'd'*:8,9-*b''c''d''*:12,13-*b'''c'''d'''*]tetrafuran, $C_{24}H_8O_4$

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(*Received* 14 *February* 1983; *accepted* 13 *May* 1983)

Abstract. $M_r = 360{\cdot}4$, monoclinic, $P2_1/c$, $a = 3{\cdot}745\,(1)$, $b = 11{\cdot}602\,(3)$, $c = 16{\cdot}597\,(3)$ Å, $\beta = 93{\cdot}87\,(2)°$, $V = 719{\cdot}5\,(5)$ Å^3, $Z = 2$, $D_x = 1{\cdot}664\,(1)$ Mg m^{-3}, μ(Cu $K\alpha$) = 0·61 mm^{-1}, $F(000) = 368$. The final R value is 0·068 for 491 observed independent reflexions, collected using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) at room temperature and for which $I_{\rm net} \geq 4\sigma(I_{\rm net})$. The molecule is planar within experimental errors. The packing is dense with a packing coefficient of 0·75.

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* Part III: Karlsson, Pilotti & Söderholm (1980).

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Introduction. Quinones frequently undergo polymerization reactions under the influence of strong acids forming complex dibenzofuran derivatives (Berg, Erdtman, Högberg, Karlsson, Pilotti & Söderholm, 1977). 1,4-Naphthoquinones and a number of 2,3-dialkylquinones have been found to give dimers, trimers and cyclic tetramers containing dibenzofuran elements. The purpose of this investigation, within a program of crystal structure studies of condensation products of quinones (Berg, Karlsson, Pilotti & Söderholm, 1978, 1980; Karlsson, Pilotti & Söderholm, 1980, 1983), is to establish whether the title compound is planar, or saddle- or boat-shaped.

Experimental. Philips PW1100 diffractometer, graphite monochromatized Cu $K\alpha$ radiation, $\theta/2\theta$ scan technique. Due to the difficulties in finding non-twinned crystals, a thin needle of dimensions 0·5 x 0·025 x 0·025 mm was used. Unit-cell parameters by least squares from 2θ values of 23 reflexions. 1380 unique reflexions out to $\theta = 65°$ $[0 \le h \le 4,\ 0 \le k \le 13$ and $|l| \le 19]$. Three reference reflexions measured every 90 min (no significant changes). Lorentz and polarization corrections, no absorption correction. Because of the relative smallness and low scattering power of the specimen only the highest amplitudes could be reliably measured. Hence only 491 reflexions satisfied the criterion $I_{\rm net} > 4\sigma(I_{\rm net})$.

Direct methods [*MULTAN* (Germain, Main & Woolfson, 1971)], full-matrix least-squares refinement based on $|F|$, with the weighting scheme of Hughes (1941): $|F_{o,\,\rm min}| = 3{\cdot}0$; final $R = 0{\cdot}068$ $wR = 0{\cdot}083$, S value = 0·083. H atoms from a difference map. In the final cycles of refinement the C and O atoms were assigned anisotropic temperature factors, the temperature factor for each H atom being fixed to the $B_{\rm iso}$ of the carrier atom. $\Delta/\sigma = 0{\cdot}05$ in final cycle. In final difference map $-0{\cdot}3 \le \Delta\rho \le 0{\cdot}3$ e Å^{-3}. The atomic scattering factors of Freeman (1959) were used for the non-hydrogens, and those of Stewart, Davidson & Simpson (1965) for the hydrogens.

Table 1. *Positional parameters* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å^2) *for the non-hydrogen atoms*

Coordinates for the atoms centrosymmetrically related to those listed here are derived by use of the operator $-x$, $-y$, $1-z$.

	x	y	z	B
C(1)	1251 (22)	−3538 (8)	5538 (6)	4·5 (3)
C(2)	2423 (20)	−3519 (8)	4765 (5)	4·3 (2)
C(2a)	2370 (17)	−2512 (7)	4343 (5)	3·5 (2)
O(3)	3452 (12)	−2311 (5)	3562 (3)	4·3 (2)
C(3a)	3013 (18)	−1146 (7)	3418 (5)	3·4 (2)
C(4)	3762 (21)	−578 (10)	2708 (5)	4·3 (3)
C(5)	3141 (20)	580 (9)	2650 (5)	4·3 (3)
C(5a)	1789 (18)	1169 (7)	3316 (5)	3·6 (3)
O(6)	1020 (14)	2324 (6)	3336 (3)	4·7 (2)
C(6a)	−212 (17)	2494 (8)	4130 (4)	3·8 (2)
C(12c)	1327 (17)	−1447 (7)	4661 (5)	3·2 (2)
C(12d)	1686 (16)	−595 (7)	4074 (4)	3·3 (2)
C(12e)	1077 (17)	586 (7)	4021 (4)	3·0 (2)
C(12f)	−157 (16)	1470 (7)	4543 (4)	3·3 (2)

Discussion. Positional parameters and $B_{\rm eq}$ values for the non-hydrogen atoms are listed in Table 1.* The molecule contains a center of symmetry, which excludes the possibility of it having either the boat or saddle form. The atom-numbering scheme and bond lengths and angles are shown in Fig. 1. Standard deviations for the bonds and angles are estimated to be 0·008–0·015 Å and 0·6–0·8°, respectively. The standard deviations in the measured bond lengths all fall within the expected range. It is noteworthy, however, that the C_{sp^2}—C_{sp^2} single bonds in the five-membered rings are shorter than reported for dibenzofuran itself: 1·480 (6) Å (Banerjee, 1973, 1974) and 1·481 (3) Å (Dideberg, Dupont & André, 1972). In all structures determined within this program of study, however, this type of bond is shortened relative to that of dibenzofuran.

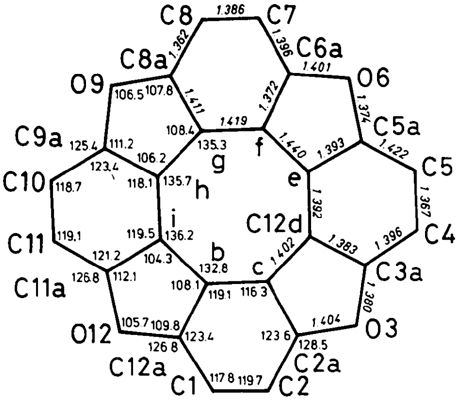

Fig. 1. Numbering scheme, bond distances (Å) and angles (°). The two halves of the molecule are related by a symmetry center.

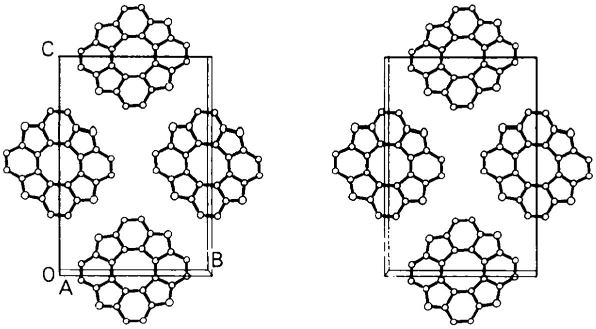

Fig. 2. A stereoscopic view (*PLUTO*78, Motherwell & Clegg, 1978) of the molecular packing.

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* Lists of anisotropic temperature factors for the non-hydrogen atoms, coordinates and isotropic temperature factors for the hydrogens and the observed and calculated structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38602 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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.

The authors are indebted to Jan-Eric Berg for stimulating discussions and also to Professor Peder Kierkegaard for his continued interest in this work. The crystals used were kindly supplied by Professor Holger Erdtman and Dr Hans-Erik Högberg.

The present research program has received financial support from the Swedish Natural Science Research Council.

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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}, $\mu(\mathrm{Cu}\ K\alpha) = 0{\cdot}73$ 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 $I_{\rm net} \geq 4\sigma(I_{\rm net})$. 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).

0108-2701/83/091275-03$01.50