for this was 1·19 Å, but experimentally determined values have a wide spread from 1·14 to 1·27 Å. The recent accurate determination of *p*-dinitrobenzene (Di Rienzo, Domenicano & Riva di Sanseverino, 1980) gave 1·218 and 1·220 (2) Å for N=O, and the electron diffraction analysis of the same structure gave 1·219 (2) Å (Sadova, Popik, Vilkov, Pankrushev & Shlyapochnikov, 1974), which agree well with our mean value of 1·220 (3) Å. It is noteworthy that in our structure one of the N—O bonds in each nitro group is longer than the other (mean values 1·233 and 1·208 Å).

In the case of the C=O bonds, that where the O accepts two hydrogen bonds is longer than the other (1·242 compared with 1·218 Å). Evidence for H(5) bonding to O(8) rather than to O(5′) is that the distance H(5)···O(8) is 1·857 (44) compared with H(5)···O(5′)=2·334 (43) Å. The direct distances O(5)···O(8) and O(6)···O(8) are 2·562 (3) and 2·569 (3) Å respectively, whereas the distances *via* the H atoms, O(5)—H(5)···O(8) and O(6)—H(6)···O(8), are 2·767 and 2·709 Å, involving angles at H(5) of 132·6 (3·5) and at H(6) of 142·4 (3·7)°.

The mean atomic deviation from the plane of the anthraquinone nucleus [atoms C(1)—C(14)] is 0·028 (2) Å. The mean deviation from the plane of nitro group C(1), N(1), O(1), O(2) is 0·005 (2) Å and from nitro group C(8), N(2), O(3), O(4) is 0·014 (2) Å. The dihedral angles between the anthraquinone nucleus and the two nitro groups are 83·83 (5) and 62·88 (5)° respectively, and the angle between the two nitro groups is 144·12 (5)°.

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2,5-Bis(1,1,3,3-tetramethylbutyl)-1,4-benzoquinone, $C_{22}H_{36}O_2$

BY C. J. BROWN AND J. E. CHANNING

Department of Metallurgy and Materials Engineering, City of London Polytechnic, Central House, Whitechapel High Street, London E1 7PF, England

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Abstract. $M_r = 332·52$, monoclinic, $P2_1/a$, $a = 11·912$ (12), $b = 15·586$ (12), $c = 6·542$ (10) Å, $\beta = 119·37$ (10)°, $V = 1058·48$ Å^3, $D_x = 1·043$, $D_m = 1·035$ Mg m^{-3}, $Z = 2$, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 0·50 mm^{-1}, $F(000) = 368$, $R = 0·060$ for 723 observed [$I > 3\sigma(I)$] reflexions. The structure comprises discrete centrosymmetrical molecules with no strong intermolecular forces.

Introduction. The material supplied by Kodak Limited was known to be diisooctylbenzoquinone, and one reason for undertaking this work was to determine which of the 80 or more octyl isomers was present. Another reason was the relative scarcity of accurate structural data on quinones.

Experimental. Golden-yellow acicular crystals (m.p. 411 K) from aqueous ethanol solution, elemental analysis gave C 79·50, H 10·80% (required for $C_{22}H_{36}O_2$, C 79·50, H 10·80%); unit-cell dimensions obtained initially from rotation photographs and more accurately from 2θ measurements on Weissenberg photographs, intensity data obtained by the multiple-film technique and visual comparison of densities with a calibrated scale on photographs about **c** (0–5 levels), inter-layer scaling and cross-correlation made using a zero-level **b** Weissenberg photograph; 1166 measured reflexions; data reduction and structure determination carried out using the NRC suite of programs (Ahmed, 1970) on the ICL 1905E computer at the London Polytechnics Computer Unit; the E map obtained from 135 reflexions with $E \geq 1·5$ showed all the non-H atoms; positional parameters, together with isotropic temperature factors, starting from the Wilson-plot value ($B = 2·86$ Å^2), refined by least squares to $R = 0·10$; weights $w = 1/F_o$; H atoms, obtained by a combination

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Table 1. *Final atomic parameters and e.s.d.'s*

$B_{eq} = \frac{4}{3}\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
C(1)	0·0555 (5)	0·0397 (3)	−0·1159 (8)	3·97 (9)
C(2)	0·1248 (4)	0·0449 (3)	0·1448 (8)	4·04 (9)
C(3)	0·0678 (4)	0·0050 (3)	0·2418 (7)	3·76 (9)
C(4)	0·2554 (4)	0·0894 (3)	0·2749 (8)	4·23 (9)
C(5)	0·3492 (5)	0·0415 (4)	0·2127 (10)	5·47 (12)
C(6)	0·3144 (5)	0·0779 (3)	0·5339 (10)	5·80 (12)
C(7)	0·2553 (5)	0·1836 (3)	0·2053 (9)	4·29 (10)
C(8)	0·1639 (5)	0·2534 (3)	0·2163 (9)	4·92 (11)
C(9)	0·2041 (7)	0·3388 (5)	0·1607 (14)	7·62 (17)
C(10)	0·1678 (9)	0·2602 (5)	0·4566 (14)	8·45 (17)
C(11)	0·0236 (7)	0·2395 (4)	0·0201 (13)	7·37 (16)
O(1)	0·0984 (3)	0·0755 (2)	−0·2348 (6)	5·63 (8)

Table 2. *Bond lengths* (Å) *and bond angles* (°)

C(1)–C(3′)	1·462 (8)	C(4)–C(7)	1·538 (7)
C(1)–C(2)	1·488 (6)	C(7)–C(8)	1·566 (8)
C(2)–C(3)	1·293 (7)	C(8)–C(9)	1·519 (9)
C(2)–C(4)	1·525 (7)	C(8)–C(10)	1·553 (11)
C(4)–C(5)	1·554 (8)	C(8)–C(11)	1·544 (10)
C(4)–C(6)	1·493 (7)	C(1)–O(1)	1·252 (7)
C(3′)–C(1)–C(2)	120·8 (4)	C(5)–C(4)–C(6)	103·9 (4)
C(3′)–C(1)–O(1)	117·8 (5)	C(5)–C(4)–C(7)	106·1 (4)
C(2)–C(1)–O(1)	121·4 (5)	C(6)–C(4)–C(7)	112·5 (4)
C(1)–C(2)–C(3)	114·0 (4)	C(4)–C(7)–C(8)	123·3 (4)
C(1)–C(2)–C(4)	120·3 (4)	C(7)–C(8)–C(9)	106·8 (5)
C(3)–C(2)–C(4)	125·6 (4)	C(7)–C(8)–C(10)	114·7 (5)
C(2)–C(3)–C(1′)	125·2 (5)	C(7)–C(8)–C(11)	111·0 (5)
C(2)–C(4)–C(5)	107·7 (4)	C(9)–C(8)–C(10)	109·0 (6)
C(2)–C(4)–C(6)	111·2 (4)	C(9)–C(8)–C(11)	105·3 (5)
C(2)–C(4)–C(7)	114·6 (4)	C(10)–C(8)–C(11)	109·5 (6)

of difference Fourier maps and torsion-angle calculations, introduced into the structure factor calculations but not refined; anisotropic temperature factor refinement for the non-H atoms also commenced at this stage; refinement terminated when all shifts were $< 0{\cdot}3\ \sigma$ and $R = 0{\cdot}060$, $R_w = 0{\cdot}095$; scattering factors from *International Tables for X-ray Crystallography* (1962).

Discussion. The final positional and isotropic thermal parameters for the non-H atoms are listed in Table 1.* The numbering of the atoms used in this analysis together with the disposition of the molecules in the unit cell are shown in Fig. 1. The configuration of the octyl group is 1,1,3,3-tetramethylbutyl which was confirmed by an NMR spectral analysis carried out by Dr D. Jopling of the Kodak Research Laboratories. The integrated peak areas agreed with the numbers of CH_2 and CH_3 groups which we found, and the essential features of the spectrum agreed with those of the model reference compound 2,4,4-trimethyl-2-(*p*-hydroxyphenyl)pentane.

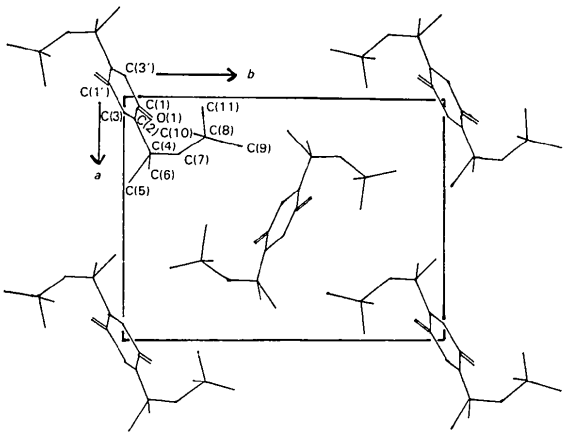

Fig. 1. Projection of contents of unit cell on (001). Primed atoms are related to the corresponding unprimed ones by the centre of symmetry at (0,0,0).

The bond lengths and interbond angles resulting from the refinement are given in Table 2. There are no intermolecular contacts shorter than 3·8 Å between non-H atoms.

O(1) and C(4) deviate by 0·007 (4) and −0·086 (5) Å from the mean plane of the quinone ring. The mean aliphatic C—C distance is 1·536 Å. The dimensions of the quinone ring vary somewhat from those in related compounds:

	C(1)–C(2)	C(2)–C(3)	C(1)–C(3)	C(1)–O(1)
p-Benzoquinone (Trotter, 1960)	1·447 Å	1·322 Å	1·477 Å	1·222 Å
2,5-Dimethyl-1,4-benzoquinone (Hirshfeld & Rabinovich, 1967)	1·502	1·347	1·482	1·223
Title compound	1·488 (6)	1·293 (7)	1·462 (8)	1·252 (7)

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38217 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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