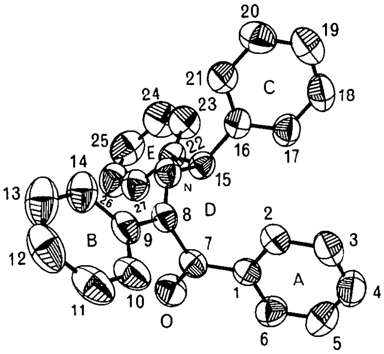

Fig. 1. An *ORTEP* view of the molecule with the atomic numbering.

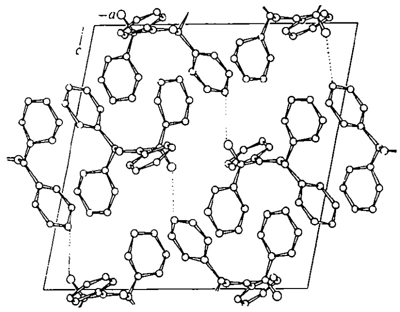

Fig. 2. The molecular packing viewed down **b**. Dotted lines indicate intermolecular distances less than 3·5 Å [3·483 (3) Å].

Table 6. *Selected torsion angles* (°)

C(2)–C(1)–C(7)–C(8)	1·3 (2)	C(7)–C(8)–C(9)–C(10)	24·6 (2)
C(6)–C(1)–C(7)–O	1·9 (3)	C(7)–C(8) N· C(15)	−3·4 (2)
C(1)–C(7)–C(8)–N	81·2 (3)	C(16)–C(15)–N–C(8)	112·3 (2)
C(1)–C(7)–C(8)–C(9)	−102·7 (2)	C(22)–C(15)–N- C(8)	−122·5 (2)
O–C(7)–C(8)–N	−98·0 (2)	N–C(15)–C(16)–C(21)	137·0 (2)
O–C(7)–C(8)–C(9)	78·2 (2)	N–C(15)–C(22)–C(23)	133·0 (2)

Table 7. *Dihedral angles* (°)

$A \wedge B$	90·4 (1)	$B \wedge E$	68·6 (1)	$B \wedge D$	22·8 (1)
$B \wedge C$	100·2 (1)	$C \wedge E$	95·2 (1)	$C \wedge D$	86·5 (1)
$A \wedge E$	24·0 (1)	$A \wedge D$	78·8 (1)	$E \wedge D$	54·9 (1)
$B \wedge C$	103·8 (1)				

the molecule is distorted from planarity. The dihedral angles between the planes through the different parts of the molecule are listed in Table 7. Packing of the molecules in the unit cell is shown in Fig. 2; the intermolecular distance C(25)—O less than 3·5 Å (3·483 Å) is marked by the dotted line; the structure is stabilized by van der Waals interactions.

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1,4,5,8-Naphthalenetetrone

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Abstract. $C_{10}H_4O_4$, monoclinic, $P2_1/n$, $a = 6{\cdot}510\ (4)$, $b = 13{\cdot}220\ (5)$, $c = 4{\cdot}855\ (4)$ Å, $\beta = 110{\cdot}0\ (5)$°, $D_x = 1{\cdot}592$ g cm^{-3} for $Z = 2$. The compound crystallizes as yellow needles. The structure was refined to $R_F = 0{\cdot}07$, using 1102 I measured on a four-circle diffractometer (Mo $K\alpha$). The molecules have (almost exactly) $2/m$ symmetry, with the twofold axis along C(9)—C(10); the carbonyl oxygens are displaced by ±0·265 Å from the plane through the central six C atoms. The molecular shape differs overall from that of

the nitrogen analogue pyridazino[1,2-*a*]pyridazine-1,4,5,8-tetrone [Laing, Sommerville & Piacenza (1977), *Acta Cryst.* B**33**, 2464–2471], which has approximate symmetry 222 (D_2).

Introduction. 1,4,5,8-Naphthalenetetrone, synthesized from naphthazarin by oxidation with lead tetraacetate (Zahn & Ochwat, 1928), is a very powerful oxidizing agent and Lewis acid. It is therefore of interest as a potential electron acceptor in the formation of donor–acceptor charge-transfer molecular compounds; in addition the propinquity of the carbonyl oxygens is likely to lead to distortion of the molecular framework from planarity, as has already been reported for the nitrogen analogue pyridazino[1,2-*a*]pyridazine-1,4,5,8-tetrone (DIAZAN) (Laing, Sommerville & Piacenza, 1977).

Yellow crystals were obtained by the method of Zahn & Ochwat (1928); although moisture must be rigorously excluded during the preparation, the crystals are stable in the atmosphere. After preliminary photography, cell dimensions (see *Abstract*) and intensities of 1197 unique reflections were measured on a Philips PW 1100 four-circle diffractometer (graphite-monochromated Mo $K\alpha$), using the $\omega/2\theta$ method. The crystal was stable in the X-ray beam. Absorption corrections were not applied. The structure was solved by direct methods and refined using *SHELX* 77; 1102 reflections were included in the final refinement stage (90 'zero-value' reflections and 5 with registration errors were omitted). The weighting scheme was $w(F_o) = 0{\cdot}5174/[\sigma(F_o) + 0{\cdot}000496\,F_o^2]$; $R_F = 0{\cdot}07$ and $R_w = 0{\cdot}065$. Atomic parameters are in Table 1.*

Bond lengths, angles and deviations from planarity are given in Fig. 1. Although the molecular symmetry is $\bar{1}$ (C_i), averaging of values in accord with symmetry $2/m$ (C_{2h}) is justified, the twofold axis running along C(9)—C(10). The molecules are arranged in stacks, with approximate close packing of the quasi-cylindrical stacks (Fig. 2). There are no intermolecular approaches less than standard van der Waals distances.

Table 1. *Atomic coordinates, with equivalent isotropic temperature factors for nonhydrogen atoms and isotropic temperature factors for* H *atoms*

$U_{eq} = \frac{1}{3}\,\text{trace}\,\mathbf{U}$.

	x	y	z	U_{eq} or U_{iso} (Å^2)
C(1)	0·4152 (3)	0·3607 (1)	−0·0950 (3)	0·0342 (8)
C(2)	0·5928 (3)	0·3276 (1)	−0·1982 (4)	0·0412 (9)
C(7)	0·2651 (3)	0·6073 (1)	0·2376 (4)	0·0414 (9)
C(8)	0·2783 (2)	0·4984 (1)	0·1818 (3)	0·0331 (8)
C(9)	0·4275 (2)	0·4669 (1)	0·0202 (3)	0·0299 (7)
O(1)	0·2618 (2)	0·3055 (1)	−0·1138 (3)	0·0531 (8)
O(4)	0·1785 (2)	0·4374 (1)	0·2748 (3)	0·0493 (7)
HC(2)	0·597 (3)	0·258 (2)	−0·242 (4)	0·042 (5)
HC(7)	0·160 (3)	0·626 (2)	0·327 (4)	0·050 (6)

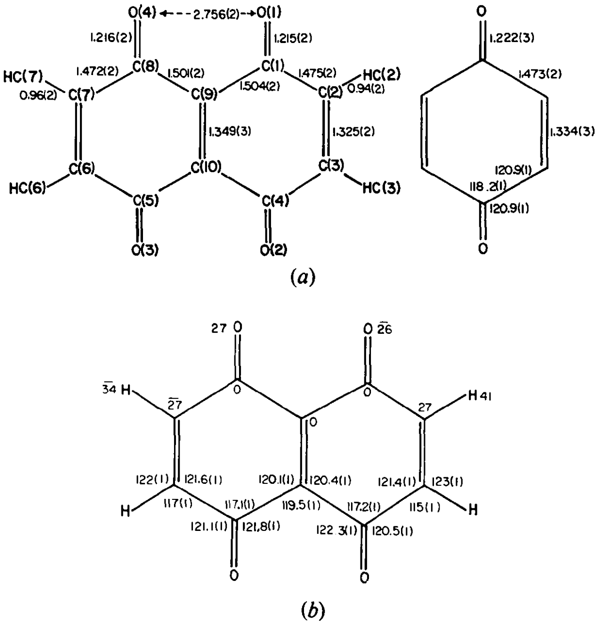

Fig. 1. (*a*) Numbering of atoms and bond lengths (Å). (*b*) Bond angles (°) and deviations (units of 10^{-2} Å) of atoms from the best plane through the six central C atoms. The equation of this plane is: $0{\cdot}6835X - 0{\cdot}2917Y + 0{\cdot}6691Z + 0{\cdot}5830$ (Å) $= 0$ where $X \parallel \mathbf{a}^*$, $Y \parallel (\mathbf{c} \times \mathbf{a}^*)$, $Z \parallel \mathbf{c}$. The e.s.d.'s of the deviations from the best plane are ~0·002 Å for C, O and ~0·03 Å for H. Dimensions of *p*-benzoquinone at 113 K (van Bolhuis & Kiers, 1978) are shown for comparison.

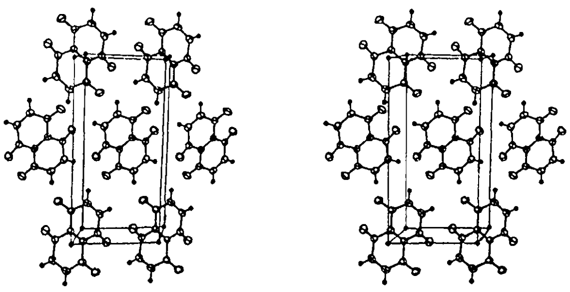

Fig. 2. *ORTEP* (Johnson, 1965) stereodiagram of the molecular packing in 1,4,5,8-naphthalenetetrone. The origin is at the rear lower left corner of the unit cell and the axes run as follows: *a* horizontal, *b* vertical, *c* inclined by 70° to the page.

Discussion. The molecule is a tetraquinone, essentially without conjugation between the several double bonds. A rather similar result has been obtained for DIAZAN. Bond lengths and angles agree well with those in *p*-benzoquinone at 113 K (van Bolhuis & Kiers, 1978).

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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 38022 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

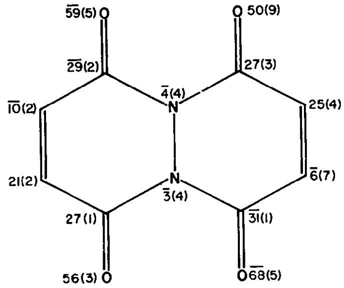

Fig. 3. Geometry of DIAZAN (Laing, Sommerville & Piacenza, 1977) averaged over chemically equivalent parameters for the three crystallographically independent molecules in the unit cell ($P2_1/c$, $Z = 12$). The e.s.d.'s in brackets [$(N - 1)$ e.s.d.'s where N is the sample size] refer to the measured values and it seems probable that the main contributions to the e.s.d.'s come from real differences between the independent molecules. (Deviations are in units of 10^{-2} Å).

Table 2. *Modes of deformation of naphthalenes symmetrically substituted in the* 1,4,5,8 *positions* (*symmetries are only approximate for some molecules*)

Type 1 – deformation to 222 symmetry	
1,4,5,8-Tetrachloronaphthalene	(Davydova & Struchkov, 1962; Gafner & Herbstein, 1962)
1,4,5,8-Tetrabromonaphthalene	(Davydova & Struchkov, 1968)
1,5-Dibromo-4,8-dichloronaphthalene	(Davydova & Struchkov, 1965)
Octamethylnaphthalene	(Hart, 1978; Sim, 1982)
Octachloronaphthalene	(Herbstein, 1979)
Tetrabenznaphthalene (dibenzo[*g*,*p*]chrysene)	(Herbstein, 1979)
5,6-Dichloro-11,12-diphenylnaphthacene	(Avoyan, Kitaigorodsky & Struchkov, 1964)
DIAZAN	(Laing, Sommerville & Piacenza, 1977)
Type 2 – deformation to 2/*m* symmetry	
1,4,5,8-Tetranitronaphthalene (form II)	(Holden & Dickinson, 1969)
1,4,5,8-Tetraphenylnaphthalene	(Evrard, Piret & Van Meerssche, 1972)
1,4,5,8-Naphthalenetetrone	(present paper)

Reduction of angle C(6)—C(5)—C(10) by 2–3° below 120° seems to be a standard feature in aromatic quinones. In the present compound and in DIAZAN the carbonyl groups are displaced principally up and down, and the sideways displacement found in the *peri*-substituted naphthalenes [as shown by the increase of angles O(4)—C(8)—C(9) and C(9)—C(1)—O(1) above 120°] occurs only to a minor extent. (Fig. 3 shows the geometry of DIAZAN averaged over the three crystallographically independent molecules in the unit cell.)

Most naphthalenes (or analogues) which are symmetrically substituted in the 1,4,5,8 positions and suffer from *peri* strain deform to a shape with 222 (D_2) symmetry, but there are now three examples with $2/m$ (C_{2h}) symmetry (Table 2). The details of the deformation of the rings in these three molecules differ: in 1,4,5,8-tetranitronaphthalene the naphthalene ring system is almost planar (largest displacement 0·05 Å), while in the present molecule the central six carbons are coplanar with C(2) displaced by 0·27 Å; in 1,4,5,8-tetraphenylnaphthalene each six-membered ring has a boat conformation.

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