Hull, Lessinger, Germain, Declercq & Woolfson, 1978), non-H atoms refined on F using full-matrix least squares with *SHELX* (Sheldrick, 1976), H atoms found in difference Fourier map, refined with isotropic temperature factors equal to those of their bonded C atoms; refinement of overall scale factor, positional and thermal parameters (anisotropic for non-hydrogen atoms) converged to $R = 0{\cdot}060$ for 1272 reflections (index range h 0 to 9, k 0 to 16, l 0 to 22; $\sin\theta \le 0{\cdot}39$); unit weights used throughout refinement; max. Δ in final LS cycle = $1{\cdot}1\sigma$, $\Delta\rho = \pm 0{\cdot}4$ e Å^{-3}; scattering factors from *SHELX*.

Discussion. Atomic coordinates are listed in Table 1* and bond angles in Table 2. The labelling of the atoms in the molecule and the bond lengths are shown in Fig. 1. The packing of the molecules viewed along **a** is illustrated in Fig. 2. Fig. 3 is an *ORTEP* (Johnson, 1965) drawing of the molecule; the conformation is defined by the torsion angles.* The phenyl ring is planar, the algebraic sum of the ring torsion angles being 0·08°. The chlorophenyl ring is also nearly planar. The average deviation of the atoms from the least-squares plane is 0·032 Å with the chlorine included, and 0·027 Å without it. The dihedral angle between the planes of the two phenyl rings is −150·3 (2)° and that between the chlorophenyl ring and the heterocyclic ring is 53·3 (4)°. S(2) and the exocyclic atoms bonded to it show a significant departure from the plane. The oxathiazine ring, containing two double bonds, exhibits a distorted half-chair conformation. There are no intermolecular contacts shorter than the sums of the van der Waals radii. The crystal structure therefore contains discrete molecules.

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* Lists of structure factors, anisotropic thermal parameters, bond angles involving H atoms and torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39242 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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9,10-Dihydro-9,10-epidioxyanthracene, $C_{14}H_{10}O_2$

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Abstract. $M_r = 210{\cdot}23$, monoclinic, $P2_1/a$, $a = 15{\cdot}944\,(10)$, $b = 5{\cdot}863\,(10)$, $c = 11{\cdot}432\,(10)$ Å, $\beta = 108{\cdot}2\,(2)°$, $V = 1015{\cdot}20$ Å^3, $Z = 4$, $D_m = 1{\cdot}356\,(4)$, $D_x = 1{\cdot}375$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}75$ mm^{-1}, $F(000) = 440$, $T = 293$ K, $R = 0{\cdot}062$ for 798 observed reflexions [$I > 3\sigma(I)$]. Molecules in the crystal are discrete and held together by van der Waals forces. The intramolecular dimensions are normal for anthraquinone-type compounds. The two benzo rings make a dihedral angle of 52·66 (5)°.

Introduction. A dilute solution of anthracene in carbon disulphide forms a peroxide when irradiated with ultra-violet light; crystals of the title compound are deposited on evaporation of the solvent (Dufraisse & Gérard, 1935). These crystals are stable over long periods in a corked phial in a refrigerator or in a cool room, but decompose in a few hours at elevated temperature or in an X-ray beam forming a mixture of anthrone and anthraquinone (Lonsdale, Nave & Stephens, 1966). The decomposition is explosive at the

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melting point (440 K). This structure determination was undertaken to understand better the *in situ* solid-state change.

Experimental. Crystals ~2·0 × 0·2 × 0·2 mm by recrystallization from ethanol, fresh crystal used for each layer in a series of multiple-film Weissenberg photographs $h0l \rightarrow h5l$, $hk0 \rightarrow hk3$ and $0kl$. Density by flotation in NaI solution, lattice parameters from rotation photographs and more accurately from a least-squares fit to 15 2θ measurements on Weissenberg photographs, $\theta_{\max} = 55°$, visual estimation of intensities by comparison with a calibrated scale, data scaled and cross-correlated, corrections for Lp effects but not for absorption or extinction, index range h 0–19, k 0–6, l −12 to +10, 798 reflexions observed out of a possible 1023. Structure determined by trial-and-error, noting particularly strong reflexions $F(40\bar{2})$ and $F(14,0,0)$, refinement by least squares on F using Cruickshank & Pilling's (1961) programs on the Pegasus computer at University College, and later using the *NRC* programs (Ahmed, Hall, Pippy & Huber, 1970). Initially, C and O atoms refined using B_{iso}, and finally B_{ij}, weights $w^{1/2} = 1/F_o$; H atoms derived by calculation, included in structure-factor calculations with $B_{\text{iso}} = 9{\cdot}0$ Å^2 and not refined. Attempts at refining H resulted in a lower R factor but less consistent molecular geometry; final shifts $< 0{\cdot}3\sigma$, $\Delta\rho$ in final difference Fourier map $\pm 0{\cdot}1$ e Å^{-3}, scattering factors from *International Tables for X-ray Crystallography* (1962), $R = 0{\cdot}062$, $R_w = 0{\cdot}15$ for 798 reflexions.

Table 1. *Atomic parameters and e.s.d.'s*

$$B_{\text{eq}} = \tfrac{4}{3}(\beta_{11}/a^{*2} + \beta_{22}/b^{*2} + \beta_{33}/c^{*2}).$$

	x	y	z	B_{eq}(Å^2)
C(1)	0·2908 (5)	0·6166 (11)	0·1153 (6)	7·85 (14)
C(2)	0·2127 (4)	0·5514 (14)	0·1300 (7)	8·27 (14)
C(3)	0·2024 (4)	0·3504 (13)	0·1890 (6)	7·87 (12)
C(4)	0·2752 (4)	0·2104 (11)	0·2335 (6)	7·62 (12)
C(5)	0·5675 (4)	0·2451 (11)	0·4476 (7)	7·45 (12)
C(6)	0·6329 (4)	0·3976 (13)	0·5024 (6)	8·21 (13)
C(7)	0·6414 (4)	0·5964 (15)	0·4401 (7)	8·88 (14)
C(8)	0·5849 (4)	0·6471 (13)	0·3237 (8)	9·23 (14)
C(9)	0·4515 (4)	0·5075 (12)	0·1447 (8)	8·09 (14)
C(10)	0·4412 (4)	0·1420 (12)	0·2501 (8)	8·50 (15)
C(11)	0·5118 (4)	0·2966 (12)	0·3321 (6)	7·52 (13)
C(12)	0·5192 (3)	0·4929 (11)	0·2708 (6)	6·60 (11)
C(13)	0·3611 (4)	0·4721 (10)	0·1590 (6)	7·25 (12)
C(14)	0·3542 (4)	0·2712 (11)	0·2190 (5)	6·90 (12)
O(1)	0·4687 (3)	0·3090 (8)	0·0761 (4)	9·13 (9)
O(2)	0·4630 (3)	0·0896 (8)	0·1365 (4)	8·50 (9)

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

C(1)–C(2)	1·362 (8)	C(9)–C(12)	1·510 (8)
C(1)–C(13)	1·369 (8)	C(9)–C(13)	1·516 (9)
C(2)–C(3)	1·393 (9)	C(9)–O(1)	1·476 (7)
C(3)–C(4)	1·383 (8)	C(10)–C(11)	1·519 (8)
C(4)–C(14)	1·368 (8)	C(10)–C(14)	1·522 (8)
C(5)–C(6)	1·368 (8)	C(10)–O(2)	1·478 (8)
C(5)–C(11)	1·375 (8)	C(11)–C(12)	1·372 (8)
C(6)–C(7)	1·394 (9)	C(13)–C(14)	1·384 (7)
C(7)–C(8)	1·386 (9)	O(1)–O(2)	1·476 (5)
C(8)–C(12)	1·373 (8)		
C(2)–C(1)–C(13)	117·2 (5)	C(5)–C(11)–C(10)	126·4 (5)
C(1)–C(2)–C(3)	123·2 (5)	C(5)–C(11)–C(12)	122·8 (5)
C(2)–C(3)–C(4)	117·8 (5)	C(10)–C(11)–C(12)	110·5 (5)
C(3)–C(4)–C(14)	120·0 (5)	C(8)–C(12)–C(9)	127·0 (5)
C(6)–C(5)–C(11)	117·9 (5)	C(8)–C(12)–C(11)	120·2 (5)
C(5)–C(6)–C(7)	119·6 (6)	C(9)–C(12)–C(11)	112·7 (5)
C(6)–C(7)–C(8)	122·2 (6)	C(1)–C(13)–C(9)	125·0 (5)
C(7)–C(8)–C(12)	117·3 (6)	C(1)–C(13)–C(14)	121·7 (5)
C(12)–C(9)–C(13)	108·0 (5)	C(9)–C(13)–C(14)	113·3 (5)
C(12)–C(9)–O(1)	105·5 (4)	C(4)–C(14)–C(10)	130·4 (5)
C(13)–C(9)–O(1)	106·8 (5)	C(4)–C(14)–C(13)	120·0 (5)
C(11)–C(10)–C(14)	107·0 (5)	C(10)–C(14)–C(13)	109·4 (5)
C(11)–C(10)–O(2)	109·6 (5)	C(9)–O(1)–O(2)	113·0 (4)
C(14)–C(10)–O(2)	110·2 (5)	C(10)–O(2)–O(1)	107·2 (4)

Discussion. The numbering of the atoms and packing of the molecules in the unit cell are shown in Fig. 1.* Final atomic parameters are in Table 1, and bond lengths and inter-bond angles in Table 2. The intramolecular dimensions are normal for anthraquinone-type compounds, the mean aromatic C—C bond being 1·377 (8) Å, and the mean C—C single bond 1·517 (8) Å. There are 50 intermolecular distances < 4·0 Å between non-H atoms, the shortest being between O(1) atoms across the centre of symmetry, 3·182 (5) Å. The two benzo rings make a dihedral angle of 52·66 (5)°. The solid-state decomposition into anthrone and anthraquinone has been fully discussed in the paper by Lonsdale *et al.* (1966).

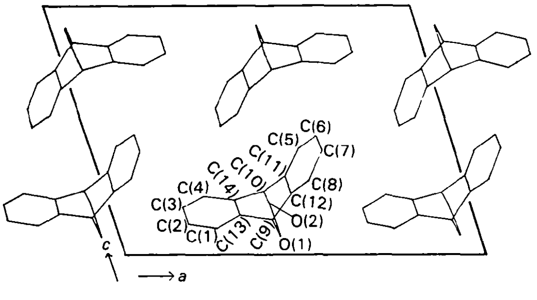

Fig. 1. Numbering of atoms and packing of molecules.

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* Lists of structure factors, H-atom parameters, intermolecular distances, mean-plane equations and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39266 (10 pp.). Copies may be obtained through The executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.