Table 2. *Bond distances* (Å) *and angles* (°)

E.s.d.'s are given in parentheses.

	A	*B*
N(1)–C(2)	1·36 (1)	1·37 (1)
N(1)–C(6)	1·37 (1)	1·38 (1)
N(1)–C(7)	1·49 (1)	1·50 (1)
C(2)–O(2)	1·219 (9)	1·23 (1)
C(2)–N(3)	1·37 (1)	1·38 (1)
N(3)–C(4)	1·37 (1)	1·39 (1)
C(4)–O(4)	1·243 (9)	1·21 (1)
C(4)–C(5)	1·46 (1)	1·45 (1)
C(5)–C(5*m*)	1·50 (1)	1·51 (1)
C(5)–C(6)	1·34 (1)	1·34 (1)
C(7)–C(8)	1·52 (1)	1·51 (1)
C(8)–C(9)	1·50 (1)	1·53 (1)
C(9)–N(9)	1·33 (1)	1·32 (1)
C(9)–O(9)	1·23 (1)	1·24 (1)
C(2)–N(1)–C(6)	121·2 (6)	120·9 (6)
C(2)–N(1)–C(7)	118·7 (6)	118·8 (6)
C(6)–N(1)–C(7)	120·1 (6)	120·3 (6)
N(1)–C(2)–O(2)	122·1 (6)	122·2 (7)
N(1)–C(2)–N(3)	115·5 (6)	115·3 (6)
O(2)–C(2)–N(3)	122·5 (6)	122·6 (7)
C(2)–N(3)–C(4)	126·6 (6)	126·9 (6)
N(3)–C(4)–O(4)	120·8 (6)	119·5 (7)
N(3)–C(4)–C(5)	115·7 (6)	114·6 (7)
O(4)–C(4)–C(5)	123·5 (6)	125·9 (7)
C(4)–C(5)–C(5*m*)	118·5 (6)	118·4 (7)
C(4)–C(5)–C(6)	116·9 (7)	118·4 (7)
C(5*m*)–C(5)–C(6)	124·6 (7)	123·2 (7)
N(1)–C(6)–C(5)	124·0 (7)	123·9 (7)
N(1)–C(7)–C(8)	111·4 (6)	111·0 (6)
C(7)–C(8)–C(9)	112·4 (6)	113·4 (6)
C(8)–C(9)–N(9)	116·6 (6)	117·1 (6)
C(8)–C(9)–O(9)	122·3 (7)	121·8 (7)
N(9)–C(9)–O(9)	121·7 (7)	121·1 (7)

N(1)–C(7)–C(8) are 76·7 (8) and −80·7 (8)°, N(1)–C(7)–C(8)–C(9) 61·7 (8) and −72·0 (8)°, C(7)–C(8)–C(9)–O(9) 52 (1) and −34 (1)°, and C(7)–C(8)–C(9)–N(9) −127·0 (7) and 145·8 (7)°, for *A* and *B*, respectively.

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Structure of 3-(2-Hydroxy-4-methylphenyl)-3-phenylphthalide

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Abstract. $C_{21}H_{16}O_3$, $M_r = 316{\cdot}36$, monoclinic, $P2_1/n$, $a = 8{\cdot}099\,(2)$, $b = 11{\cdot}178\,(3)$, $c = 18{\cdot}524\,(6)$ Å, $\beta = 99{\cdot}01\,(2)°$, $V = 1656{\cdot}3\,(8)$ Å^3, $Z = 4$, $D_m = 1{\cdot}26$, $D_x = 1{\cdot}268$ Mg m^{-3}, $\lambda(\text{Mo}\,K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}091$ mm^{-1}, $F(000) = 664$, $T = 293$ K. Final $R = 0{\cdot}037$ for 1514 unique observed reflections. The geometry of the five-membered ring is generally comparable to other γ-lactones. The tetrahedral symmetry at the central tetra-substituted C atom is distorted by its association with the fused-ring system and by the overcrowding in this molecule, the valence angles range from 101·8 (2) to 113·9 (2)°. The packing is determined by an intermolecular hydrogen bond between the hydroxyl and carbonyl groups with an O···O distance of 2·758 (3) Å and an O—H···O angle of 170 (3)°.

Introduction. 3,3-Diarylphthalides display laxative properties (Loewe & Hubacher, 1941; Hubacher, Doernberg & Horner, 1953) and serve as the sub-

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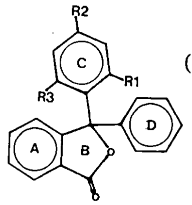
strates for 9-acetoxy-10-arylanthracenes. In both cases these compounds must be homogeneous and pure, but frequently their synthesis gives a mixture of isomers, of which only one is biologically active. For instance, phenolphthalein exhibits laxative potency in contrast to isophenolphthalein, which is inactive (Hubacher *et al.*, 1953).

The new title compound (I) has recently been synthesized by Professor Gronowska, Department of Organic Chemistry, N. Copernicus University, Toruń, by the condensation of 2-benzoylbenzoic acid with *m*-cresol. During this reaction two isomers were obtained: 3-(2-hydroxy-4-methylphenyl)-3-phenylphthalide [(I), 36%] and 3-(4-hydroxy-2-methylphenyl)-3-phenylphthalide [(II), 51%]. Previously it was reported (Dutt, 1940; Rumiński, 1973) that only isomer (II) was obtained in this reaction.



(I) $R1 = \mathrm{OH}$, $R2 = \mathrm{Me}$, $R3 = \mathrm{H}$
(II) $R1 = \mathrm{Me}$, $R2 = \mathrm{OH}$, $R3 = \mathrm{H}$
(III) $R1 = \mathrm{Me}$, $R2 = \mathrm{H}$, $R3 = \mathrm{OH}$

Isomers (I) and (II) have different melting points and only isomer (I) undergoes cyclization and acetylation to form the appropriate 9-acetoxy-10-phenylanthracene derivative. The X-ray crystallographic study of these isomers has been undertaken in order to confirm their chemical structure, to explain why the isomer (III) is not formed and to obtain more information on the relationships between structure and reactivity. The last two points will be discussed in a later paper together with the structure of isomer (II).

Experimental. Colourless crystals of (I) grown from ethanol solution by slow evaporation, m.p. 487·5–488·7 K; density measured by flotation in aqueous KI solution; crystal specimen: 0·30 × 0·30 × 0·26 mm in sealed glass capillary on Enraf–Nonius CAD-4 diffractometer, ω–2θ scan mode with graphite-monochromated Mo $K\alpha$ radiation; accurate cell parameters refined from setting angles of 20 reflections with $20 < 2\theta < 30°$; max. $(\sin\theta)/\lambda = 0\cdot5946$ Å^{-1}, $-9 \le h \le 9$, $0 \le k \le 13$, $0 \le l \le 21$; three intensity standards (34$\bar{2}$, 309, 128) displayed no significant variation; 2912 unique reflections measured, 1398 unobserved reflections $(I < 2\sigma_I)$; no absorption correction.

Solution by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982); full-matrix least-squares refinement using F magnitudes with *SDP* package (Enraf–Nonius, 1982); all H atoms located on difference Fourier maps and refined isotropically; anisotropic displacement parameters for non-H atoms; 281 parameters refined.

Final $R = 0\cdot037$, $wR = 0\cdot037$ ($w^{-1} = \sigma_F^2$) and $S = 0\cdot78$ for 1514 observed reflections; max. $(\Delta/\sigma) = 0\cdot52$ in final cycle; peaks in final ΔF map within $\pm0\cdot16$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Other computer programs used: *ORTEP*II (Johnson, 1976), *PLUTO* (Motherwell & Clegg, 1978) and the *CRYPOZ* system (Jaskólski, 1982).

Discussion. The final atomic parameters for non-H atoms are given in Table 1.* Bond lengths, bond angles and selected torsion angles are listed in Table 2. A perspective view of the molecule with the atom-numbering scheme is shown in Fig. 1.

Bond distances and angles in the five-membered ring (*B*) agree in general with the values found in other γ-lactones (Carpy, Feniou, Naifi & Colleter, 1984; Kalyani & Vijayan, 1969). In the lactone group, bond-length asymmetry is observed. The two formally single C—O bonds: C(1)—O(1) and O(1)—C(2) differ by 0·130 Å, in good agreement with values reported in similar structures (Jeffrey, Rosenstein & Vlase, 1967; Kim, Jeffrey, Rosenstein & Corfield, 1967; Fridrichsons & Mathieson, 1962; Kalyani & Vijayan, 1969; Carpy *et al.*, 1984) and is a result of the different hybridization state of atoms C(1) and C(2).

The average C—C bond lengths in the two phenyl rings *C* and *D* are 1·385 (3) and 1·380 (3) Å, respectively. The corresponding value in the six-membered ring *A* of the phthalide system is 1·382 (3) Å. The closing of the two chemically equivalent angles C(4)—C(5)—C(6) and C(3)—C(8)—C(7) to 117·4 (3) and 117·5 (3)° is usual in structures where the benzene ring is fused to a smaller ring (Allen, 1981).

The tetrahedral angular symmetry at C(1) is distorted by the association of this atom with the five-membered ring and by overcrowding in the molecule: the largest deviations from 109·5° are 101·8 (2) and 113·9 (2)°. The arrangement of the *ortho*-substituted phenyl ring *C*, with the torsion angle C(4)—C(1)—C(15)—C(20) close to zero, results in almost equal distances between atom O(3) and atoms O(1) and C(9) [2·890 (3) and 2·878 (4) Å, respectively] and between atoms C(20) and C(4) [2·894 (5) Å].

The fused-ring system is not exactly planar, having a dihedral angle of 2·8 (3)° between rings *A* and *B*. The least-squares planes of the phenyl rings *C* and *D* form angles 104·8 (3) and 110·5 (3)° with the plane of ring

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44408 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

A and an angle of 81·5 (3)° between themselves. When the whole molecule is treated as a distorted propeller with an axis along C(1)–O(1), the angles between the planes of rings *A*, *C* and *D* and the appropriate O(1)–C(1)–C(Ph) planes are 4·2 (3), 64·8 (3) and 21·0 (3)°. Such an arrangement results in a short intramolecular contact of 2·39 (2) Å between atoms H(C10) and O(1). According to Taylor & Kennard (1982), this distance as well as the other geometrical features of this contact [C(10)···O(1) = 2·797 (4), C(10)–H(C10) = 1·01 (2) Å and C(10)–H(C10)···O(1) = 103 (1)°] are in the ranges observed for C–H···O hydrogen bonds. However, this could also be a result of intramolecular constraints in the molecule.

The packing of the molecules (Fig. 2) in the crystal is determined by the intermolecular H bond formed between the hydroxyl group O(3)–H(O3) and the carbonyl O(2^{i}) atom of an adjacent lactone group [(i) $\frac{3}{2}-x$, $\frac{1}{2}+y$, $\frac{1}{2}-z$]. Hydrogen-bond geometry: $O_D\cdots O_A = 2{\cdot}758\ (3)$, $O_D{-}H = 0{\cdot}74\ (4)$, $O_A\cdots H = 2{\cdot}02\ (4)$ Å, $O_D{-}H\cdots O_A = 170\ (3)$°.

Table 1. *Atomic fractional coordinates and equivalent isotropic displacement parameters* (Å^2) *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	U_{eq}
C(1)	0·5908 (3)	0·2848 (3)	0·3847 (1)	0·0393 (8)
C(2)	0·7612 (4)	0·1151 (3)	0·3880 (2)	0·0491 (9)
C(3)	0·7069 (4)	0·1240 (3)	0·4594 (2)	0·0445 (9)
C(4)	0·6031 (4)	0·2220 (3)	0·4581 (1)	0·0409 (8)
C(5)	0·5268 (4)	0·2487 (3)	0·5185 (2)	0·0551 (9)
C(6)	0·5625 (4)	0·1747 (4)	0·5791 (2)	0·066 (1)
C(7)	0·6689 (5)	0·0788 (3)	0·5802 (2)	0·066 (1)
C(8)	0·7419 (4)	0·0506 (3)	0·5203 (2)	0·061 (1)
C(9)	0·4109 (3)	0·2866 (3)	0·3461 (1)	0·0423 (8)
C(10)	0·3444 (4)	0·1949 (3)	0·3006 (2)	0·0548 (9)
C(11)	0·1766 (5)	0·1956 (4)	0·2708 (2)	0·073 (1)
C(12)	0·0742 (4)	0·2871 (4)	0·2862 (2)	0·079 (1)
C(13)	0·1401 (4)	0·3790 (4)	0·3301 (2)	0·075 (1)
C(14)	0·3086 (4)	0·3798 (3)	0·3603 (2)	0·060 (1)
C(15)	0·6760 (3)	0·4065 (3)	0·3886 (2)	0·0384 (8)
C(16)	0·6840 (4)	0·4708 (3)	0·3245 (2)	0·0426 (8)
C(17)	0·7632 (4)	0·5803 (3)	0·3271 (2)	0·0483 (9)
C(18)	0·8385 (4)	0·6297 (3)	0·3926 (2)	0·0495 (9)
C(19)	0·8293 (4)	0·5671 (3)	0·4565 (2)	0·0504 (9)
C(20)	0·7503 (4)	0·4573 (3)	0·4537 (2)	0·0439 (9)
C(21)	0·9289 (5)	0·7472 (3)	0·3952 (2)	0·085 (1)
O(1)	0·6906 (2)	0·2046 (2)	0·34454 (9)	0·0437 (5)
O(2)	0·8516 (3)	0·0423 (2)	0·3661 (1)	0·0688 (8)
O(3)	0·6132 (3)	0·4205 (2)	0·2601 (1)	0·0594 (6)

Table 2. *Bond lengths* (Å), *bond angles and selected torsion angles* (°) *with e.s.d.'s in parentheses*

C(1)–O(1)	1·483 (3)	C(9)–C(14)	1·382 (4)
C(1)–C(4)	1·520 (3)	C(10)–C(11)	1·384 (5)
C(1)–C(9)	1·519 (3)	C(11)–C(12)	1·375 (6)
C(1)–C(15)	1·522 (5)	C(12)–C(13)	1·366 (6)
C(2)–O(1)	1·353 (4)	C(13)–C(14)	1·391 (5)
C(2)–O(2)	1·207 (4)	C(15)–C(16)	1·398 (5)
C(2)–C(3)	1·463 (5)	C(15)–C(20)	1·383 (5)
C(3)–C(4)	1·379 (5)	C(16)–C(17)	1·379 (5)
C(3)–C(8)	1·386 (5)	C(16)–O(3)	1·362 (4)
C(4)–C(5)	1·393 (4)	C(17)–C(18)	1·385 (5)
C(5)–C(6)	1·388 (5)	C(18)–C(19)	1·387 (5)
C(6)–C(7)	1·374 (5)	C(18)–C(21)	1·501 (5)
C(7)–C(8)	1·373 (5)	C(19)–C(20)	1·381 (5)
C(9)–C(10)	1·382 (4)		

C(4)–C(1)–C(9)	110·5 (2)	C(1)–C(9)–C(10)	122·1 (2)
C(4)–C(1)–C(15)	113·9 (2)	C(1)–C(9)–C(14)	118·7 (2)
C(4)–C(1)–O(1)	101·8 (2)	C(10)–C(9)–C(14)	119·2 (3)
C(9)–C(1)–C(15)	113·9 (2)	C(9)–C(10)–C(11)	120·2 (3)
C(9)–C(1)–O(1)	109·3 (2)	C(10)–C(11)–C(12)	120·5 (3)
C(15)–C(1)–O(1)	106·6 (2)	C(11)–C(12)–C(13)	119·4 (3)
C(1)–O(1)–C(2)	111·2 (2)	C(12)–C(13)–C(14)	120·8 (3)
C(3)–C(2)–O(1)	109·2 (3)	C(13)–C(14)–C(9)	119·9 (3)
C(3)–C(2)–O(2)	129·4 (3)	C(1)–C(15)–C(16)	120·0 (2)
O(1)–C(2)–O(2)	121·4 (2)	C(1)–C(15)–C(20)	122·7 (2)
C(2)–C(3)–C(4)	107·8 (2)	C(16)–C(15)–C(20)	117·2 (3)
C(2)–C(3)–C(8)	130·0 (3)	C(15)–C(16)–C(17)	120·6 (3)
C(4)–C(3)–C(8)	122·1 (3)	C(15)–C(16)–O(3)	117·6 (3)
C(1)–C(4)–C(3)	109·8 (2)	C(17)–C(16)–O(3)	121·8 (3)
C(1)–C(4)–C(5)	130·1 (2)	C(16)–C(17)–C(18)	121·5 (3)
C(3)–C(4)–C(5)	120·1 (3)	C(17)–C(18)–C(19)	118·1 (3)
C(4)–C(5)–C(6)	117·4 (3)	C(17)–C(18)–C(21)	121·5 (3)
C(5)–C(6)–C(7)	121·9 (3)	C(19)–C(18)–C(21)	120·3 (3)
C(6)–C(7)–C(8)	121·0 (3)	C(18)–C(19)–C(20)	120·2 (3)
C(7)–C(8)–C(3)	117·5 (3)	C(19)–C(20)–C(15)	122·2 (3)

O(1)–C(1)–C(9)–C(10)	22·6 (3)	C(4)–C(1)–C(15)–C(16)	175·8 (3)
O(1)–C(1)–C(9)–C(14)	−161·0 (3)	C(4)–C(1)–C(15)–C(20)	−3·0 (3)
O(1)–C(1)–C(15)–C(16)	64·3 (3)	C(9)–C(1)–C(15)–C(16)	−56·2 (3)
O(1)–C(1)–C(15)–C(20)	−114·5 (3)	C(9)–C(1)–C(15)–C(20)	124·9 (3)
C(4)–C(1)–C(9)–C(10)	−88·7 (3)	C(15)–C(1)–C(9)–C(10)	141·6 (3)
C(4)–C(1)–C(9)–C(14)	87·7 (3)	C(15)–C(1)–C(9)–C(14)	−42·0 (3)

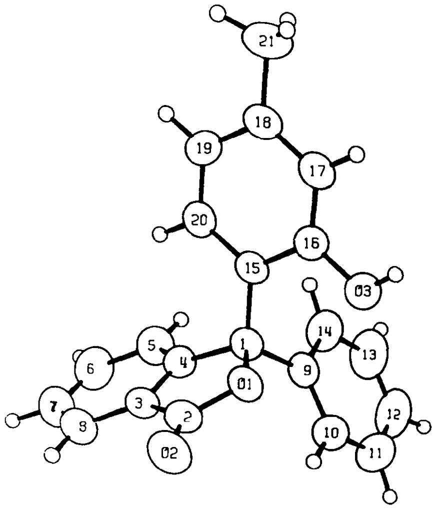

Fig. 1. Perspective view of the molecule with atom-numbering scheme. Thermal ellipsoids are shown at the 50% probability level, H atoms as small spheres of arbitrary size.

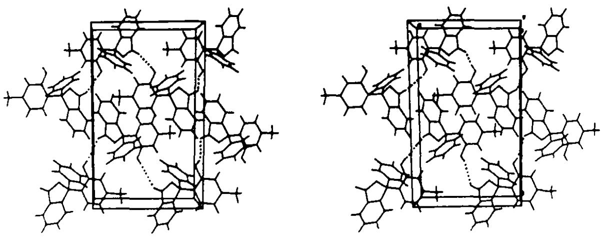

Fig. 2. Stereoview of the crystal structure projected along **a**. Hydrogen bonds are indicated by dotted lines.

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Structure of 9-Acetoxy-10-(2-acetoxy-4-ethylphenyl)anthracene

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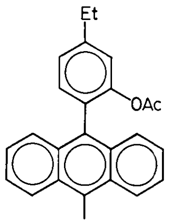
Abstract. 10-(2-Acetoxy-4-ethylphenyl)-9-anthryl acetate, $C_{26}H_{22}O_4$, $M_r = 398{\cdot}46$, triclinic, $P\bar{1}$, $a = 8{\cdot}835\,(2)$, $b = 13{\cdot}903\,(3)$, $c = 8{\cdot}577\,(2)$ Å, $\alpha = 96{\cdot}33\,(2)$, $\beta = 94{\cdot}71\,(2)$, $\gamma = 96{\cdot}66\,(2)°$, $V = 1035{\cdot}2\,(4)$ Å^3, $Z = 2$, $D_x = 1{\cdot}278$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 0{\cdot}61$ mm^{-1}, $F(000) = 420$, $T = 293$ K. Final $R = 0{\cdot}045$ for 2526 unique observed reflections. The molecular geometry is generally similar to that exhibited by other 9-acetoxy-10-arylanthracenes. The anthracene and phenyl rings exhibit deformations consistent with the σ-electron characteristics of their substituents. The dihedral angle between the phenyl ring and the anthracene system [69·2 (3)°] is sensitive to phenyl-ring substitution and may have a bearing on the fluorescence properties of compounds in this series.

Introduction. The structure of the title compound (I) was determined as part of investigations on 9-acetoxy-10-arylanthracenes, which all exhibit marked fluorescence in organic solvents (Gronowska, Aleksandrzak & Heldt, 1981) and are used as active media for dye lasers (Heldt, 1983). It was found (Heldt, 1983) that compounds having 2-acetoxy substitution of the 10-phenyl ring show laser activity different from the others, probably due to the electronic interaction of this group with the π system of anthracene.



(I)

X-ray structural studies of 9-acetoxy-10-(2-acetoxy-5-bromophenyl)anthracene (II) (Roszak & Skrzat, 1985) and 9-acetoxy-10-(2,4-diacetoxyphenyl)anthracene (III) (Roszak & Borowiak, 1986) have shown different positions of the 2′-OAc group in relation to anthracene. In the two independent molecules of (II) the

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