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

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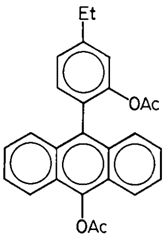
**Abstract.** 10-(2-Acetoxy-4-ethylphenyl)-9-anthryl acetate, $C_{26}H_{22}O_4$, $M_r = 398{\cdot}46$, triclinic, $P\bar{1}$, $a = 8{\cdot}835\,(2)$, $b = 13{\cdot}903\,(3)$, $c = 8{\cdot}577\,(2)$ Å, $\alpha = 96{\cdot}33\,(2)$, $\beta = 94{\cdot}71\,(2)$, $\gamma = 96{\cdot}66\,(2)°$, $V = 1035{\cdot}2\,(4)$ Å$^3$, $Z = 2$, $D_x = 1{\cdot}278$ Mg m$^{-3}$, $\lambda$(Cu $K\alpha$) $= 1{\cdot}54178$ 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 $\sigma$-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 $\pi$ 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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Table 1. *Atomic fractional coordinates and equivalent isotropic displacement parameters* (Å²) *with e.s.d.'s in parentheses*

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

| | $x$ | $y$ | $z$ | $U_{\text{eq}}$ |
|---|---|---|---|---|
| C(1) | 0·9429 (2) | 0·3933 (2) | 1·1241 (3) | 0·0562 (7) |
| C(2) | 0·9376 (3) | 0·4245 (2) | 1·2782 (3) | 0·0650 (8) |
| C(3) | 0·8142 (3) | 0·3906 (2) | 1·3589 (3) | 0·0633 (8) |
| C(4) | 0·6956 (2) | 0·3279 (1) | 1·2838 (2) | 0·0506 (7) |
| C(5) | 0·4431 (2) | 0·1424 (1) | 0·7835 (2) | 0·0504 (7) |
| C(6) | 0·4476 (3) | 0·1148 (2) | 0·6271 (2) | 0·0600 (8) |
| C(7) | 0·5774 (3) | 0·1437 (2) | 0·5511 (2) | 0·0635 (8) |
| C(8) | 0·6995 (3) | 0·1993 (2) | 0·6309 (2) | 0·0565 (7) |
| C(9) | 0·8216 (2) | 0·2923 (1) | 0·8807 (2) | 0·0455 (6) |
| C(10) | 0·5680 (2) | 0·2312 (1) | 1·0374 (2) | 0·0409 (6) |
| C(11) | 0·5703 (2) | 0·2009 (1) | 0·8748 (2) | 0·0427 (6) |
| C(12) | 0·7007 (2) | 0·2311 (1) | 0·7952 (2) | 0·0450 (6) |
| C(13) | 0·8209 (2) | 0·3268 (1) | 1·0397 (2) | 0·0442 (6) |
| C(14) | 0·6918 (2) | 0·2944 (1) | 1·1193 (2) | 0·0418 (6) |
| C(15) | 0·4346 (2) | 0·1947 (1) | 1·1191 (2) | 0·0419 (6) |
| C(16) | 0·3285 (2) | 0·2535 (1) | 1·1715 (2) | 0·0459 (6) |
| C(17) | 0·1995 (2) | 0·2169 (2) | 1·2364 (3) | 0·0562 (7) |
| C(18) | 0·1726 (3) | 0·1190 (2) | 1·2548 (2) | 0·0567 (7) |
| C(19) | 0·2792 (3) | 0·0593 (1) | 1·2059 (2) | 0·0567 (7) |
| C(20) | 0·4067 (2) | 0·0966 (1) | 1·1403 (2) | 0·0500 (7) |
| C(21) | 1·0588 (3) | 0·2708 (2) | 0·7810 (3) | 0·0630 (8) |
| C(22) | 1·1829 (3) | 0·3218 (2) | 0·7017 (4) | 0·0945 (12) |
| C(23) | 0·3658 (3) | 0·4224 (2) | 1·2716 (3) | 0·0626 (8) |
| C(24) | 0·4039 (4) | 0·5210 (2) | 1·2230 (4) | 0·0907 (11) |
| C(25) | 0·0292 (4) | 0·0787 (2) | 1·3225 (4) | 0·0887 (11) |
| C(26) | −0·1105 (4) | 0·0726 (3) | 1·2138 (5) | 0·1150 (15) |
| O(1) | 0·9454 (2) | 0·3283 (1) | 0·8021 (2) | 0·0563 (5) |
| O(2) | 1·0533 (2) | 0·1917 (1) | 0·8223 (3) | 0·0943 (8) |
| O(3) | 0·3521 (2) | 0·3525 (1) | 1·1452 (2) | 0·0562 (5) |
| O(4) | 0·3518 (2) | 0·4046 (1) | 1·4027 (2) | 0·0881 (7) |

acetoxy group twists away from the anthracene system and out of its preferred position perpendicular to the phenyl ring (Hummel, Roszak & Bürgi, 1987), while in (III) it twists by 23·2(4)° towards the anthracene system and adopts a distinctive orientation with the C=O bond parallel to the long axis of anthracene. These different arrangements may result from the differing influences of the other substituents on the phenyl ring (Roszak, 1986); however, further crystal structures of other related compounds are required to substantiate this supposition.

**Experimental.** Light-brown parallelepipeds of (I) were grown from acetic acid by slow evaporation; crystal system and approximate cell dimensions determined from Weissenberg and oscillation photographs; crystal size: 0·40 × 0·25 × 0·40 mm; Syntex $P2_1$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation, $\theta$–$2\theta$ scan mode, background and intensity of reflections calculated by peak-profile analysis (Lehmann & Larsen, 1974); accurate cell parameters refined from setting angles of 15 reflections with $31 \le 2\theta \le 49°$; max. $(\sin\theta)/\lambda = 0{\cdot}5461$ Å$^{-1}$; $-9 \le h \le 9$, $-15 \le k \le 15$, $0 \le l \le 9$; two intensity standards [$\bar{3}11$: 823 (6); $\bar{1}0\bar{4}$: 926 (7)]; 2977 reflections measured, 2769 unique ($R_{\text{int}} = 0{\cdot}0183$), 243 unobserved ($I < 1{\cdot}96\sigma_I$); no absorption correction.

Solution by direct methods in $P1$ (origin-positioning problem in $P\bar{1}$) using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), space group $P\bar{1}$ justified by $E$ statistics and successful (full-matrix) refinement with *SHELX*76 (Sheldrick, 1976) using $F$ magnitudes; all H atoms except those from methyl groups located on difference Fourier maps, methyl groups initially treated as rigid groups with tetrahedral geometry and C—H distances of 1·08 Å, finally all H-atom parameters fixed, non-H atoms refined anisotropically, 272 parameters refined. Final $R = 0{\cdot}045$, $wR = 0{\cdot}071$ (weighting scheme $w^{-1} = \sigma^2 + 0{\cdot}00006F^2$) and $S = 5{\cdot}42$ for 2526 observed reflections; empirical isotropic extinction parameter $x$ (*SHELX*76, Sheldrick, 1976) converged at 0·012 (3); $(\Delta/\sigma)_{\text{max}} = 0{\cdot}012$ in last cycle, $(\Delta\rho)_{\text{max}} = 0{\cdot}22$ and $(\Delta\rho)_{\text{min}} = -0{\cdot}19$ e Å$^{-3}$ in final $\Delta F$ map; atomic 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.* The molecular geometry

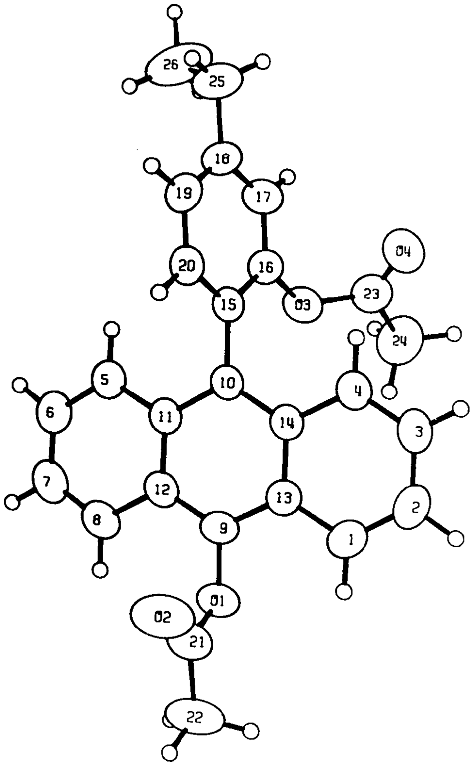

Fig. 1. Perspective view of the molecule with atom-numbering scheme. Thermal ellipsoids are shown at the 50% probability level and H atoms as small spheres of arbitrary size.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44409 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

with atom-numbering scheme is shown in Fig. 1. Bond lengths and bond angles are listed in Table 2; they are very similar to those for other 9-acetoxy-10-aryl-anthracenes (Roszak & Skrzat, 1985; Roszak & Borowiak, 1986; Roszak & Duax, 1987; Roszak & Borowiak, 1987).

The anthracene ring system as a whole, and its three individual rings, are not strictly planar. The dihedral angle between the least-squares planes of the outer rings is 4·8 (3)°. The phenyl ring forms a dihedral angle of 69·2 (3)° with the anthracene system. In (II) this angle was 69·9 (4) and 64·8 (4)° (in the two independent molecules) and 68·2 (3)° in (III). However, in other related compounds which lack a 2-substituent on the 10-phenyl ring, this angle increases to 84·4 (1)° in 9-acetoxy-10-(4-acetoxyphenyl)anthracene (Roszak & Duax, 1987) and to 74·0 (4), 79·7 (4) and 73·0 (4)° in the three molecules of 9-acetoxy-10-phenylanthracene (Roszak & Borowiak, 1987). This suggests that the 2′-OAc substituent influences the phenyl–anthracene arrangement in compounds (I), (II) and (III).

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

| | | | |
|---|---|---|---|
| C(1)—C(13) | 1·426 (3) | C(13)—C(14) | 1·431 (3) |
| C(1)—C(2) | 1·351 (3) | C(15)—C(16) | 1·384 (3) |
| C(2)—C(3) | 1·403 (3) | C(15)—C(20) | 1·393 (3) |
| C(3)—C(4) | 1·351 (3) | C(16)—C(17) | 1·379 (3) |
| C(4)—C(14) | 1·432 (3) | C(16)—O(3) | 1·413 (2) |
| C(5)—C(11) | 1·429 (3) | C(17)—C(18) | 1·384 (3) |
| C(5)—C(6) | 1·359 (3) | C(18)—C(19) | 1·385 (3) |
| C(6)—C(7) | 1·406 (3) | C(18)—C(25) | 1·512 (3) |
| C(7)—C(8) | 1·341 (3) | C(19)—C(20) | 1·373 (3) |
| C(8)—C(12) | 1·429 (3) | C(21)—C(22) | 1·489 (3) |
| C(9)—C(12) | 1·388 (3) | C(21)—O(1) | 1·363 (3) |
| C(9)—C(13) | 1·396 (3) | C(21)—O(2) | 1·189 (3) |
| C(9)—O(1) | 1·403 (2) | C(23)—C(24) | 1·487 (3) |
| C(10)—C(11) | 1·414 (3) | C(23)—O(3) | 1·362 (3) |
| C(10)—C(14) | 1·406 (3) | C(23)—O(4) | 1·191 (3) |
| C(10)—C(15) | 1·487 (3) | C(25)—C(26) | 1·472 (5) |
| C(11)—C(12) | 1·431 (3) | | |

| | | | |
|---|---|---|---|
| C(13)—C(1)—C(2) | 120·4 (2) | C(4)—C(14)—C(13) | 117·4 (2) |
| C(1)—C(2)—C(3) | 120·8 (2) | C(10)—C(14)—C(13) | 120·4 (2) |
| C(2)—C(3)—C(4) | 120·9 (2) | C(10)—C(15)—C(16) | 123·0 (2) |
| C(3)—C(4)—C(14) | 121·1 (2) | C(10)—C(15)—C(20) | 120·7 (2) |
| C(11)—C(5)—C(6) | 120·9 (2) | C(16)—C(15)—C(20) | 116·3 (2) |
| C(5)—C(6)—C(7) | 120·7 (2) | C(15)—C(16)—C(17) | 122·2 (2) |
| C(6)—C(7)—C(8) | 120·8 (2) | C(15)—C(16)—O(3) | 116·9 (2) |
| C(7)—C(8)—C(12) | 120·9 (2) | C(17)—C(16)—O(3) | 120·8 (2) |
| C(12)—C(9)—C(13) | 123·1 (2) | C(16)—C(17)—C(18) | 120·7 (2) |
| C(12)—C(9)—O(1) | 119·1 (2) | C(17)—C(18)—C(19) | 117·9 (2) |
| C(13)—C(9)—O(1) | 117·6 (2) | C(17)—C(18)—C(25) | 120·6 (2) |
| C(11)—C(10)—C(14) | 119·7 (2) | C(19)—C(18)—C(25) | 121·5 (2) |
| C(11)—C(10)—C(15) | 119·2 (2) | C(18)—C(19)—C(20) | 120·8 (2) |
| C(14)—C(10)—C(15) | 121·2 (2) | C(19)—C(20)—C(15) | 122·1 (2) |
| C(5)—C(11)—C(10) | 122·0 (2) | O(1)—C(21)—C(22) | 110·2 (2) |
| C(5)—C(11)—C(12) | 117·8 (2) | O(2)—C(21)—C(22) | 127·4 (2) |
| C(10)—C(11)—C(12) | 120·3 (2) | O(1)—C(21)—O(2) | 122·4 (2) |
| C(8)—C(12)—C(9) | 122·7 (2) | O(3)—C(23)—C(24) | 110·8 (2) |
| C(8)—C(12)—C(11) | 118·9 (2) | O(4)—C(23)—C(24) | 125·9 (2) |
| C(9)—C(12)—C(11) | 118·3 (2) | O(3)—C(23)—O(4) | 123·3 (2) |
| C(1)—C(13)—C(9) | 122·4 (2) | C(18)—C(25)—C(26) | 113·5 (3) |
| C(1)—C(13)—C(14) | 119·3 (2) | C(9)—O(1)—C(21) | 117·5 (2) |
| C(9)—C(13)—C(14) | 118·2 (2) | C(16)—O(3)—C(23) | 118·5 (2) |
| C(10)—C(14)—C(4) | 122·2 (2) | | |

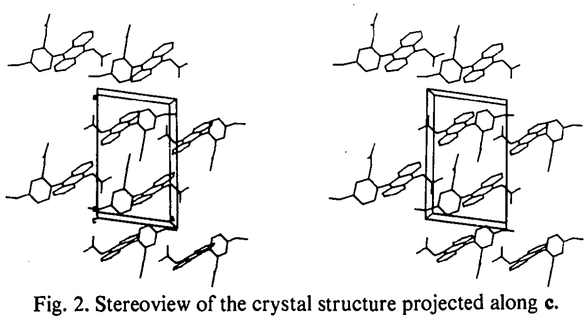

Fig. 2. Stereoview of the crystal structure projected along **c**.

The acetoxy groups are planar and their parameters are very close to the average values found for such groups (Roszak, 1986; Hummel, Roszak & Bürgi, 1987). The 9-acetoxy group is almost perpendicular to the anthracene plane [dihedral angle 82·0 (3)°]. The 2′-OAc group bonded to the 10-phenyl ring forms a dihedral angle of 58·0 (3)° with the phenyl plane and, as in (II), twists away from the anthracene plane: the torsion angle C(15)—C(16)—O(3)—C(23) is −122·3 (2)°. This angle in the two molecules of (II) was −125·6 (5) and −127·2 (5)°, while in (III) it was 69·6 (3)°.

The influence of the substituents on the internal angles of the aromatic rings in the title structure is consistent with their σ-electron character and the general theory of such substitution effects (Domenicano, Vaciago & Coulson, 1975), and very similar to effects observed in other 9-acetoxy-10-arylanthracenes (Roszak, 1986).

Fig. 2 shows the packing of molecules in the unit cell. There are no unusually short intermolecular contacts in this structure.

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# Structure of 2-(1,2-Dihydro-2,4-diphenylquinazolin-2-yl)aniline

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**Abstract.** $C_{26}H_{21}N_3$, $M_r = 375{\cdot}47$, monoclinic, $P2_1/n$ (non-standard space group), $a = 9{\cdot}3686\,(5)$, $b = 16{\cdot}8761\,(6)$, $c = 12{\cdot}4874\,(5)$ Å, $\beta = 90{\cdot}41\,(6)°$, $V = 1974{\cdot}3\,(2)$ Å$^3$, $Z = 4$, $D_x = 1{\cdot}263$ g cm$^{-3}$, $\lambda$(Cu $K\alpha$) $= 1{\cdot}54184$ Å, $\mu = 5{\cdot}47$ cm$^{-1}$, $F(000) = 792$, $T = 291$ K. Final $R = 0{\cdot}0458$ and $wR = 0{\cdot}0503$ for 2083 reflections. The 1,2-dihydroquinazoline ring system is not planar, the dihydropyrimidine ring being sofa-shaped. There is an intramolecular hydrogen bond between N3 positioned in the dihydropyrimidine ring and the amino group on the aniline moiety. This hydrogen bond elongates the phenyl–$NH_2$ bond length, and creates a sofa-shaped six-membered ring.

**Introduction.** The title compound was obtained by heating (433 K, 2 h) *o*-aminobenzophenone imine, which in turn was prepared from *o*-aminobenzonitrile and phenylmagnesium bromide as described by Bergman, Brynolf, Elman & Vuorinen (1986). The compound serves as a precursor for the preparation of phenyldibenzodiazocines. An X-ray investigation became necessary since MS, NMR and IR data did not present conclusive structural evidence.

**Experimental.** Pale yellow transparent flat prisms were obtained from an EtOH/$H_2O$ mixture. Dimensions of examined crystal were 0·40 × 0·23 × 0·15 mm. The diffraction experiment was performed using a Stoe four-circle diffractometer with Cu $K\alpha$ radiation. $\omega/2\theta$ scan with scan width 1·02° and scan speed 1·20–3·60° min$^{-1}$. Lattice parameters from least-squares refinement of setting angles of 24 reflections, $22{\cdot}04 \leq \theta \leq 29{\cdot}60°$, 3725 observations in the range $2{\cdot}62 \leq \theta \leq 69{\cdot}58°$, $-11 \leq h \leq 11$, $0 \leq k \leq 20$, $0 \leq l \leq 14$. Three standard reflections were monitored every 180, min., max. variation in intensity 2·1 and −3·6%. *SHELXS*86 (Sheldrick, 1986) was used to solve the structure. Full-matrix least-squares refinement minimizing $\sum w(\Delta F)^2$ with *SHELX*76 (Sheldrick, 1976). Non-H atoms anisotropic. All H atoms were located in difference Fourier maps, of which the three H atoms attached to nitrogens were kept and their positions isotropically refined. Remaining H atoms in their calculated geometrical positions with isotropic group temperature factors, 332 parameters refined using 2083 reflections with $F \geq 4\sigma(F)$ gave $R = 0{\cdot}0458$ and $wR = 0{\cdot}0503$, $w = 1{\cdot}0944/[\sigma^2(F) + 0{\cdot}0004F^2]$, max. $\Delta/\sigma$ for any parameter 0·001, largest and smallest density in final $\Delta F$ syntheses 0·43 and −0·13 e Å$^{-3}$. Atomic scattering factors from Cromer & Mann (1968) for C and N, and from Stewart, Davidson & Simpson (1965) for H atoms. *PARST* (Nardelli, 1983) was used for the geometrical calculations.

**Discussion.** Table 1 presents atomic coordinates and isotropic thermal parameters, Table 2 lists bond lengths and angles.* Fig. 1 shows the numbering scheme and Fig. 2 gives a stereoview of the molecule including the intramolecular hydrogen bond. Figures were drawn with *PLUTO* (Motherwell & Clegg, 1978).

The dihydroquinazoline ring system is not planar; the dihydropyrimidine ring adopts a sofa conformation, and the largest displacement from the dihydropyrimidine plane is 0·275 (3) Å (C2). The benzene ring is essentially planar but still deviates significantly from planarity; the maximum deviation is 0·009 (3) Å (C4a). The dihedral angle between these planes is 9·63 (9)°.

Bond lengths and angles in the dihydroquinazoline ring system are in fair agreement with related structures (Rogan & Williams, 1980; Hunter, Neilson & Weakley, 1985) except for N3—C4, 1·287 (3) Å. The above structures have a corresponding distance in the range 1·307—1·324 Å.

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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 44533 (41 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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