bonds [O(1*A*)—H(1*A*)$\cdots$O (*x*, *y*, *z*); O—H(1)$\cdots$O(1*A*) (2−*x*, 0·5 + *y*, 1−*z*) and O—H(2)$\cdots$O(1*B*) (2−*x*, 1·5 + *y*, 1−*z*)]. Finally, a hydrogen-bond interaction between the hydroxyl groups at C(17) of neighbouring molecules constitutes the major intermolecular attraction between 'ends' of the molecules [O(3*A*)—H(3*A*)$\cdots$O(3*B*) (*x*, *y*, *z*)]. The $D\cdots A$ lengths are, respectively 2·882 (5), 2·809 (5), 2·941 (5), 2·961 (6) and 3·166 (5) Å, H$\cdots$*A* 2·09 (5), 2·02 (4), 2·08 (4), 2·23 (5) and 2·42 (5) Å and the corresponding D—H$\cdots A$ angles are 159 (4), 148 (4), 178 (4), 161 (4) and 163 (5)°.

In addition, there are nine intramolecular C—H$\cdots$O approaches with C$\cdots$O < 3·3 Å, C(12*A*)—H(12*A*)$\cdots$O(3*A*) 2·89 (11); C(14*A*)—H(14*A*)$\cdots$O(3*A*) 2·91 (1); C(18*A*)—H(18*C*)$\cdots$O(2*A*) 3·28 (1); C(21*A*)—H(21*B*)$\cdots$O(3*A*) 2·82 (1); C(21*A*)—H(21*B*)$\cdots$O(4*A*) 2·76 (1); C(24*A*)—H(24*A*)$\cdots$O(2*A*) 2·97 (1); C(12*B*)—H(12*C*)$\cdots$O(3*B*) 2·73 (1); C(21*B*)—H(21*E*)$\cdots$O(4*B*) 2·87 (1) and C(24*B*)—H(24*C*)$\cdots$O(2*B*) 2·96 (1) Å, which stabilize the molecular conformation.

Financial support from the Consejo Nacional de Ciencia y Tecnología de México, CONACYT (Project No. PCEXECNA-040603) is acknowledged. We also tahnk Mr Abelardo Cuellar for technical assistance.

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Acta Cryst. (1987). C**43**, 1166–1168

Structure of 1,5-Bis[(4-ethylphenyl)amino]-9,10-anthracenedione

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(*Received* 27 *July* 1986; *accepted* 26 *January* 1987)

Abstract. $C_{30}H_{26}N_2O_2$, $M_r = 446·6$, monoclinic, $P2_1/c$, $a = 4·687$ (1), $b = 12·119$ (3), $c = 20·558$ (4) Å, $\beta = 93·783$ (3)°, $V = 1165·2$ Å^3, $Z = 2$, $D_x = 1·273$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 5·50$ cm^{-1}, $F(000) = 472$, $T = 297$ K, final $R = 0·0621$ for 1529 unique observed reflections. The phenyl ring is twisted by 50·3 (5)° out of the anthraquinone plane. Intramolecular hydrogen bonds are formed between the amino groups of the substituents and the carbonyl oxygens [H$\cdots$O = 1·84 (2) Å].

Introduction. The title compound (D-35, according to BDH nomenclature) belongs to a series of pleochroic dyes that were developed for application in guest–host liquid-crystal displays (Pellatt, Roe & Constant, 1980). As part of our investigations of pleochroic dyes, the molecular and crystal structures of D-35 were determined. The results are discussed in relation to the known structures of the similar dyes 1-{[4-(dimethylamino)phenyl]amino}-4-hydroxy-9,10-anthracenedione (D-27) (Foitzik, Paulus & Haase, 1986*a*), 1-{[4-(dimethylamino)phenyl]amino}-9,10-anthracenedione (D-52M) (Foitzik & Paulus, 1986), and 1,5-bis{[4-(pentyloxy)phenyl]amino}-9,10-anthracenedione (D-43) (Foitzik, Paulus & Haase, 1986*b*).

Experimental. Substance from BDH Chemicals Ltd, UK, no further purification; black–violet needles by slow evaporation of a solution in $CHCl_3$/cyclohexane; crystal dimensions 0·1 × 0·1 × 4 mm; cell constants and e.s.d.'s from least-squares refinement of 48 reflections, $29·7 < 2\theta < 58·3°$; Stoe–Stadi 4 diffractometer; 2528 intensities measured, $-1 < h < 6$, $-14 < k < 6$, $-24 < l < 24$, max. $(\sin\theta)/\lambda = 0·5617$ Å^{-1}; three standard reflections (11$\bar{4}$, 122, 1$\bar{2}$2), intensity variation <4%, 1641 unique reflections, $R_{\rm int} = 0·0160$, 112 reflections unobserved with $F_o < 2\sigma(F_o)$; no absorption correction; structure solved by direct methods with *SHELX76* (Sheldrick, 1976); most of the H atoms from difference Fourier synthesis; for comparison with the other structures of this series all C-bound H atoms placed at calculated positions (C—H = 1·08 Å), H(1N) refined; all H atoms with isotropic thermal parameters fixed at 1·1 times the average value of the diagonal

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elements of the U_{ij} matrix of the carrying atom; 161 parameters refined by least squares on F giving $R = 0{\cdot}0621$, $wR = 0{\cdot}0693$; $w = 1/\sigma^2(F_o)$; max. Δ/σ 0·03; max. $\Delta\rho$ 0·21, min. $-0{\cdot}22$ e Å^{-3} in final difference Fourier synthesis; secondary-extinction coefficient $2{\cdot}7 \times 10^{-6}$; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); all calculations performed on the IBM 3081 computer of the computing centre of the Technische Hochschule Darmstadt.

Discussion. The molecule is centrosymmetric. The atomic coordinates are listed in Table 1;* selected bond distances and angles are in Table 2.

The molecule is shown in Fig. 1. The atom-numbering scheme was chosen in accordance with that selected for the other dyes of the D-series. The angle between the best planes through the anthraquinone ring [C(1)—C(6), C(14), O(1), C($1^{\rm i}$)—C($6^{\rm i}$), C($14^{\rm i}$), O($1^{\rm i}$), where i denotes symmetry code $1-x$, $2-y$, $1-z$] and the phenyl ring is 50·3 (5)°. This is significantly different from the values of 69·5° (D-27), 73·5° (D-52M), and 75·1° (D-43) that were observed for the other dyes. These different mutual orientations of the two resonance systems may affect the spectra and especially the direction of the transition moment of the visible band. This will be discussed elsewhere (Quotschalla & Haase, 1987). Although four of the five highest peaks in the final difference Fourier synthesis are in the neighbourhood of the terminal ethylphenyl group, there is no evidence for a second position for this part of the molecule. In the crystal structures of D-27, D-43 and D-52M, the atoms C(15) and C(18) are located very close to the anthraquinone plane (max. distance 0·097 Å). In D-35 the C(15)—C(18) axis of the phenyl ring is clearly bent off that plane [deviations of 0·148 (4) and 0·291 (4) Å for C(15) and C(18), respectively].

The position of H(1N) in the anthraquinone plane and the short distance of 1·84 (2) Å to O($1^{\rm i}$) confirm the occurrence of a strong intramolecular hydrogen bond also in this dye. These hydrogen bonds are assumed to be a necessity for the light-fastness of the dyes in question in liquid-crystalline solution (Pellatt, Roe & Constant, 1980). The intramolecular hydrogen bond is also important for the formation of guest–host systems between the dye and the liquid crystal, *i.e.* for the solubility of the dye in the liquid-crystalline host (Foitzik & Haase, 1987).

Table 1. *Atomic coordinates with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å$^2 \times 10^3$)

$$U_{\rm eq} = \tfrac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{13}aa^*cc^*\cos\beta].$$

	x	y	z	$U_{\rm eq}$
C(1)	0·8844 (6)	0·8537 (2)	0·5750 (1)	64
C(2)	1·0747 (6)	0·9014 (2)	0·6226 (1)	69
C(3)	1·0708 (6)	1·0125 (2)	0·6344 (1)	71
C(4)	0·8816 (6)	1·0819 (2)	0·5999 (1)	65
C(5)	0·6958 (5)	1·0386 (2)	0·5517 (1)	58
C(6)	0·4998 (6)	1·1165 (2)	0·5151 (1)	63
C(14)	0·6935 (5)	0·9249 (2)	0·5376 (1)	57
O(1)	0·5038 (5)	1·2152 (1)	0·5316 (1)	84
N(1)	0·8854 (6)	0·7436 (2)	0·5625 (1)	78
H(1N)	0·7725 (62)	0·7249 (20)	0·5254 (12)	80*
C(15)	1·0492 (6)	0·6612 (2)	0·5960 (1)	66
C(16)	1·1912 (7)	0·5859 (2)	0·5605 (1)	81
C(17)	1·3411 (7)	0·5011 (3)	0·5911 (2)	95
C(18)	1·3616 (7)	0·4892 (2)	0·6573 (2)	85
C(19)	1·2178 (8)	0·5644 (3)	0·6927 (1)	90
C(20)	1·0600 (7)	0·6497 (2)	0·6630 (1)	85
C(27)	1·5356 (9)	0·3965 (3)	0·6906 (2)	125
C(28)	1·3794 (9)	0·2983 (3)	0·7011 (2)	131

* $U_{\rm iso}$.

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

C(1)—C(2)	1·404 (3)	C(5)—C(14)	1·407 (3)
C(1)—C(14)	1·431 (3)	C(6)—O(1)	1·242 (3)
C(1)—N(1)	1·358 (3)	N(1)—H(1N)	0·926 (25)
C(2)—C(3)	1·369 (3)	N(1)—C(15)	1·412 (3)
C(3)—C(4)	1·385 (3)	C(18)—C(27)	1·523 (4)
C(4)—C(5)	1·379 (3)	C(27)—C(28)	1·422 (4)
C(5)—C(6)	1·487 (3)		
N(1)—C(1)—C(2)	121·8 (3)	C(15)—N(1)—H(1N)	119·4 (16)
N(1)—C(1)—C(14)	120·0 (2)	C(15)—N(1)—C(1)	127·7 (2)
O(1)—C(6)—C(5)	118·4 (2)	C(16)—C(15)—N(1)	118·7 (2)
H(1N)—N(1)—C(1)	112·8 (16)	C(20)—C(15)—N(1)	122·8 (3)

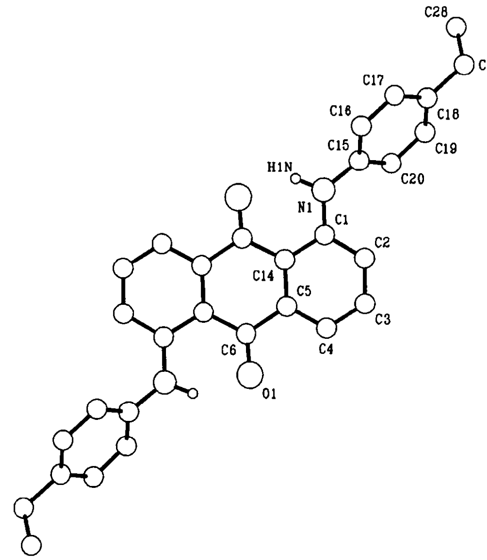

Fig. 1. The molecule with labelling scheme. H atoms except H(1N) have been omitted.

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, least-squares planes and bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43751 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

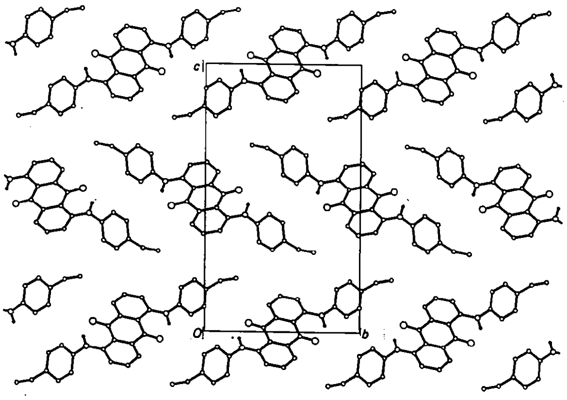

Fig. 2. Crystal structure of D-35 projected along [100].

Fig. 2 shows a projection of the crystal structure along [100]. The phenyl groups are arranged parallel to (120). The shortest distance between non-H atoms of two anthraquinone groups is 3·44 (3) Å. This is comparable with the values of 3·4–3·5 Å that were found for D-27, D-52M and D-43 and which point to slight van der Waals interactions between the aromatic systems, taking the 'van der Waals radius' as 1·85 Å (Weast, 1975). The distance between two phenyl groups related by the translation vector [100] is 3·80 (3) Å, which is significantly greater than the values of ~3·45 Å that were observed for the dyes that contain only one phenylamino substituent. For D-43 there is no close contact between the phenyl groups.

We are indebted to the Fonds der Chemischen Industrie, Frankfurt, and the Deutsche Forschungsgemeinschaft for financial support.

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Acta Cryst. (1987). C**43**, 1168–1171

Tétrabenzo[*c*,*h*,*l*,*q*]-(tétrathia-1,2,10,11 tétraaza-5,7,14,16 cyclooctadécane)

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(*Reçu le* 12 *juin* 1986, *accepté le* 27 *janvier* 1987)

Abstract. $C_{26}H_{24}N_4S_4$, $M_r = 520·8$, monoclinic, $C2/c$, $a = 16·586$ (4), $b = 9·510$ (2), $c = 15·300$ (4) Å, $\beta = 95·20$ (2)°, $V = 2403·4$ Å^3, $Z = 4$, $D_x = 1·439$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0·402$ mm^{-1}, $F(000) = 1088$, $T = 294$ (1) K, $R = 0·057$ for 792 independent reflections [$I > \sigma(I)$]. There is half a molecule per asymmetric unit. At the junction of the two halves, a C atom occupies two positions in statistical disorder. Two benzene rings are linked either by a disulfide or by a diaminomethyl group. The molecules are distributed along the $x = 0$, $x = \frac{1}{2}$ and $z = \pm\frac{1}{4}$ planes. The cohesion of the structure is due to van der Waals interactions.

Introduction. La détermination de la structure du tétrabenzo[*c*,*h*,*l*,*q*]-(tétrathia-1,2,10,11 tétraaza-5,7,-