

In contrast to the other perylenetetracarboxylic diimide pigments investigated, the single molecules of pigment (11) (Kalle AG, 1972) have no symmetry element at the centre. The flat parts of neighbouring molecules are 3.412 (38) Å apart, pack in stacks, overlap to an extent of 48.2% and are shifted against each other 27.4% longitudinally and 23.8% transversely. The two identical stacks form an angle of 87.8 (25)°. The plane of the phenyl rings is turned 71.8 (25) and 104.5 (25)° out of the plane of the perylene-imide ring system.

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## Structures of Three Perylene-3,4:9,10-bis(dicarboximide) Pigments

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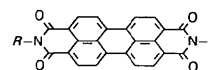
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**Abstract.** (1): *N,N'*-Dipropylperylene-3,4:9,10-bis(dicarboximide),  $C_{30}H_{22}N_2O_4$ ,  $M_r = 474.5$ , triclinic,  $P\bar{1}$ ,  $a = 18.077$  (4),  $b = 14.258$  (3),  $c = 4.689$  (3) Å,  $\alpha = 89.93$  (8),  $\beta = 111.30$  (9),  $\gamma = 104.24$  (9)°,  $V = 1086.2$  Å<sup>3</sup>,  $Z = 4$ ,  $D_m = 1.50$ ,  $D_x = 1.45$  g cm<sup>-3</sup>,  $Cu K\alpha$ ,  $\lambda = 1.54178$  Å,  $\mu = 6.93$  cm<sup>-1</sup>,  $F(000) = 496$ ,  $T = 295$  K,  $R = 6.8\%$  for 2649 reflections,  $S = 1.59$ . (2): *N,N'*-Diethylperylene-3,4:9,10-bis(dicarboximide),  $C_{28}H_{18}N_2O_4$ ,  $M_r = 446.5$ , orthorhombic,  $Pcca$ ,  $a = 34.333$  (40),  $b = 16.659$  (11),  $c = 6.906$  (2) Å,  $V = 3949.9$  Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.50$  g cm<sup>-3</sup>,  $Cu K\alpha$ ,  $\lambda = 1.54178$  Å,  $\mu = 7.84$  cm<sup>-1</sup>,  $F(000) = 1856$ ,  $T = 295$  K,  $R = 21.6\%$  for 417 reflections,  $S = 2.71$ . (3): *N,N'*-Bis(2,6-xylyl)perylene-3,4:9,10-bis(dicarboximide),  $C_{40}H_{26}N_2O_4$ ,  $M_r = 598.7$ , monoclinic,  $P2_1/c$ ,  $a = 19.929$  (15),  $b = 7.770$  (8),  $c = 25.197$  (17) Å,  $\beta = 50.42$  (8)°,  $V = 3007.2$  Å<sup>3</sup>,  $Z = 4$ ,  $D_m = 1.33$ ,  $D_x = 1.32$  g cm<sup>-3</sup>,  $Cu K\alpha$ ,  $\lambda = 1.54178$  Å,  $\mu = 6.04$  cm<sup>-1</sup>,  $F(000) = 1248$ ,  $T = 295$  K,  $R = 6.6\%$  for 3530 reflections,  $S = 1.65$ . All compounds were synthesized to verify the possible correlation between the colours of the pigments and their crystal packings. All molecules show a flat perylenetetracarboxylic diimide portion with bent side chains. The mutual arrangement of neighbours in the stacks is determined by the

substituents. The exchange of  $\pi$  electrons of these neighbours determines the different colours of the crystals.

**Introduction.** The present investigation is part of studies carried out on perylenetetracarboxylic diimide pigments (Graser & Hädicke, 1980, 1984). The crystal structures of the pigments reported here show distinct differences in their crystal packings compared with those in the preceding paper (Hädicke & Graser, 1986).



	R	Colour of crystals
(1)	CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	black
(2)	CH <sub>2</sub> -CH <sub>3</sub>	red
(3)		red

**Experimental.** All substances were recrystallized from nitrobenzene. Densities measured with a pycnometer. Crystal sizes: (1) 0.45 × 0.15 × 0.015 mm, (2) 0.20 ×

0.05 × 0.03 mm, and (3) 0.33 × 0.24 × 0.06 mm. Siemens AED diffractometer with Ni filter for (1) and (3);  $\theta/2\theta$  data collection; scan width 1.1–1.75°; five-value technique; scan rate 1–10° min<sup>-1</sup>. Syntex P2<sub>1</sub> diffractometer with graphite monochromator for (2);  $\theta/2\theta$  data collection; scan width 3.2°; scan rate 1–30° min<sup>-1</sup>. The differential scans were analysed according to an algorithm of Lehmann & Larsen (1974) (see also Blessing, Coppens & Becker, 1974) by the program *LAUSANNE* (Schwarzenbach, 1977). Lattice parameters were measured with 23 to 25 reflections up to 45° in  $\theta$ .  $(\sin\theta/\lambda)_{\max} = 0.613 \text{ \AA}^{-1}$  for (1) and (3),  $0.547 \text{ \AA}^{-1}$  for (2). Range of  $hkl$ :  $\pm h \pm k + l$  for (1),  $+h + k + l$  for (2) and  $\pm h + k + l$  for (3). Standard reflections: 1 standard reflection for each measurement [410 for (1) and 221 for (2)], monitored every 20 reflections for (1) and (3) and every 26 reflections for (2) with intensity variations (1) 7.5% and (2) 6.4%. Corrections for Lorentz and polarization but not for absorption. For (1): 4211 reflections measured and unique, 1562 unobserved [criterion  $3\sigma(F)$  and  $\overline{14,3,4, \overline{7}, 17, 11}$ ]; for (2): 2036 reflections measured and unique, 1619 unobserved [criterion  $4\sigma(F)$ ]; for (3): 5820 reflections measured and unique, 2290 unobserved [criterion  $3\sigma(F)$  and  $\overline{8, 1, 14, 17, 2, 28}$ ].

All structures were solved by direct methods using the program *SHELXTL* (Sheldrick, 1978) on a Data General Eclipse S/200 minicomputer. In the asymmetric units of all structures there are two half molecules with different conformations and packings. All molecules, except molecule (II) of (2), have an inversion centre. Molecule (II) of (2) has a twofold axis in the middle. With the program *SHELXTL* the refinement was carried out with a block-cascade algorithm. Structures (1) and (3): H atoms initially placed at calculated positions were constrained to give C–H 0.96 Å, H–C–H 109.5°, rigid CH<sub>3</sub> groups, riding CH<sub>2</sub> and CH groups with equal C–C–H angles. For C, N, and O atoms anisotropic thermal parameters were refined and for the H atoms the refinement of isotropic thermal parameters was carried out in correlated groups.

Structure (2): due to the very poor quality of the tiny crystals 417 reflections only were considered as observed ( $F > 4\sigma_F$ ) and included in the refinement. The two independent perylenetetracarboxylic diimide parts with C(13) were refined as flat rigid groups with the same geometry [C–C 1.42, C–O 1.21, N(1)–C(12) 1.39, N(1)–C(13) 1.48 Å, C–C–C 120, C(11)–N(1)–C(12) 124.5, C(11)–N(1)–C(13) 117.8°; analogous parts of both molecules are constrained in the same way]. C(14) and C(13) only were refined without constraints and gave the following bond distances and angles: C(13)–C(14) 1.512 (64), C(33)–C(34) 1.392 (76) Å, N(1)–C(13)–C(14) 122.2 (26), N(21)–C(33)–C(34) 119.9 (32)°. Only the H of the perylenetetracarboxylic diimide were included in the

refinement with the same isotropic temperature factor and with C–H bond distances of 0.96 Å and H–C–H angles of 120°. For C, N and O atoms isotropic thermal parameters were refined.

In all cases the function minimized was  $\sum w(|F_o| - |F_c|)^2$  where the weights  $w$  are calculated based on counting statistics with a term  $g$  included for random error:  $w = [\sigma^2(F) + gF^2]^{-1}$  [ $g$  for: (1) 0.00045, (2) 0.003 and (3) 0.0008]. For structure (2) the extinction was corrected with an empirical isotropic extinction parameter  $x$ , where the calculated structure factor becomes  $F_c' = F_c/(1 + xF^2/\sin 2\theta)^{1/4}$  with  $x = 22 (13) \times 10^{-7}$ . Convergences were achieved and a weighting scheme was applied to obtain a flat variance in terms of  $\sin\theta$  and the magnitude of  $F_o$ . Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). (1)  $R = 6.8\%$ ,  $wR = 6.4\%$  for 2649 reflections, (2)  $R = 21.6\%$ ,  $wR = 20.7\%$  for 417 reflections and (3)  $R = 6.6\%$ ,  $wR = 6.9\%$  for 3530 reflections.  $(\Delta/\sigma)_{\max}$  in final refinement cycle: (1) 0.1, (2) 0.003 and (3) 0.05. Max. height in final difference Fourier synthesis: (1) 0.22, (2) 0.87 and (3) 0.23 e Å<sup>-3</sup>.

Especially for structure (2) the growing of crystals was very difficult and we only obtained poor quality crystals. With the measured data of this compound we could only achieve a poor fit.

Table 1. Structure (1): atomic coordinates ( $\times 10^4$ ) and equivalent isotropic temperature factors ( $\text{\AA}^2 \times 10^3$ )

	$x$	$y$	$z$	$U_{eq}$
O(1)	2783 (2)	2192 (2)	-3958 (6)	73 (2)
O(2)	1680 (2)	4260 (2)	-442 (7)	80 (2)
N(1)	2251 (2)	3238 (2)	-2119 (7)	59 (2)
O(21)	2208 (1)	-1241 (2)	4787 (6)	63 (2)
O(22)	3502 (1)	-3615 (2)	5132 (6)	60 (1)
N(21)	2859 (2)	-2423 (2)	5012 (6)	43 (1)
C(1)	593 (2)	-150 (2)	-1266 (7)	49 (2)
C(2)	565 (2)	816 (2)	-523 (7)	47 (2)
C(3)	-15 (2)	982 (2)	697 (7)	50 (2)
C(4)	-7 (2)	1939 (3)	1329 (8)	58 (2)
C(5)	543 (2)	2719 (3)	810 (8)	60 (2)
C(6)	1109 (2)	2579 (2)	-390 (8)	54 (2)
C(7)	1122 (2)	1624 (2)	-1068 (7)	49 (2)
C(8)	1691 (2)	1470 (2)	-2331 (7)	50 (2)
C(9)	1695 (2)	535 (3)	-3040 (8)	55 (2)
C(10)	1158 (2)	-255 (3)	-2521 (7)	53 (2)
C(11)	2284 (2)	2301 (3)	-2857 (8)	59 (2)
C(12)	1684 (2)	3425 (3)	-945 (8)	60 (2)
C(13)	2822 (3)	4083 (3)	-2737 (10)	75 (3)
C(14)	3552 (3)	4580 (3)	98 (11)	82 (3)
C(15)	4092 (3)	3945 (3)	1593 (12)	112 (3)
C(21)	4382 (2)	350 (2)	627 (7)	36 (2)
C(22)	4466 (2)	-611 (2)	1276 (6)	35 (2)
C(23)	5074 (2)	-971 (2)	710 (6)	35 (2)
C(24)	5133 (2)	-1902 (2)	1483 (7)	44 (2)
C(25)	4605 (2)	-2488 (2)	2697 (7)	45 (2)
C(26)	4009 (2)	-2160 (2)	3233 (6)	38 (2)
C(27)	3934 (2)	-1214 (2)	2547 (6)	35 (2)
C(28)	3330 (2)	-866 (2)	3131 (6)	38 (2)
C(29)	3270 (2)	66 (2)	2526 (7)	43 (2)
C(30)	3782 (2)	660 (2)	1279 (7)	42 (2)
C(31)	2758 (2)	-1496 (2)	4354 (7)	45 (2)
C(32)	3456 (2)	-2798 (2)	4501 (7)	43 (2)
C(33)	2261 (2)	-3069 (2)	6084 (8)	50 (2)
C(34)	1500 (2)	-3613 (3)	3385 (8)	59 (2)
C(35)	828 (2)	-4175 (3)	4431 (10)	80 (2)

$$U_{eq} = \frac{1}{3}(\text{trace of the orthogonalized } U_{ij} \text{ matrix}).$$

**Discussion.** Tables 1–5 list final refined coordinates,  $U_{eq}$  values for the non-hydrogen atoms and the bond lengths in molecules (1)–(3).<sup>\*</sup> The atomic numbering schemes for all compounds are similar. H atoms are given the number of the C atoms to which they are attached. By way of example, Fig. 1 shows the molecular structure of (1).

<sup>\*</sup> Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond angles for the three compounds have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42365 (121 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Structure (1): bond lengths (Å)

O(1)–C(11)	1.230 (6)	O(2)–C(12)	1.217 (5)
N(1)–C(11)	1.401 (5)	N(1)–C(12)	1.404 (6)
N(1)–C(13)	1.484 (5)	O(21)–C(31)	1.219 (5)
O(22)–C(32)	1.216 (4)	N(21)–C(31)	1.397 (4)
N(21)–C(32)	1.408 (5)	N(21)–C(33)	1.474 (4)
C(1)–C(2)	1.439 (6)	C(1)–C(3')	1.471 (5)
C(1)–C(10)	1.386 (6)	C(2)–C(3)	1.428 (6)
C(2)–C(7)	1.423 (5)	C(3)–C(4)	1.392 (5)
C(4)–C(5)	1.384 (5)	C(5)–C(6)	1.387 (6)
C(6)–C(7)	1.406 (5)	C(6)–C(12)	1.476 (5)
C(7)–C(8)	1.418 (6)	C(8)–C(9)	1.376 (5)
C(8)–C(11)	1.477 (5)	C(9)–C(10)	1.380 (5)
C(13)–C(14)	1.510 (5)	C(14)–C(15)	1.482 (7)
C(21)–C(22)	1.435 (4)	C(21)–C(23')	1.470 (4)
C(21)–C(30)	1.393 (5)	C(22)–C(23)	1.426 (5)
C(22)–C(27)	1.424 (4)	C(23)–C(24)	1.396 (4)
C(24)–C(25)	1.391 (5)	C(25)–C(26)	1.374 (5)
C(26)–C(27)	1.413 (4)	C(26)–C(32)	1.471 (5)
C(27)–C(28)	1.414 (5)	C(28)–C(29)	1.381 (4)
C(28)–C(31)	1.476 (5)	C(29)–C(30)	1.386 (5)
C(33)–C(34)	1.519 (4)	C(34)–C(35)	1.521 (6)

Table 3. Structure (2): atomic coordinates ( $\times 10^4$ ) and isotropic temperature factors ( $\text{Å}^2 \times 10^3$ )

	x	y	z	U
O(1)	1372	–2203	1099	79 (16)
O(2)	1721	433	1298	74 (15)
N(1)	1558	–891	1208	41 (15)
C(1)	103	–824	99	37 (19)
C(2)	394	–225	305	13 (15)
C(3)	291	599	206	25 (16)
C(4)	583	1198	413	46 (20)
C(5)	976	972	718	52 (21)
C(6)	1079	148	816	40 (17)
C(7)	788	–451	611	62 (21)
C(8)	890	–1275	709	22 (16)
C(9)	600	–1874	503	26 (15)
C(10)	205	–1649	198	54 (22)
C(11)	1284	–1500	1014	100 (27)
C(12)	1473	–77	1122	67 (20)
C(13)	1969	–1126	1526	36 (18)
C(14)	2258 (22)	–1194 (40)	–121 (78)	64 (24)
O(21)	757	5411	881 (30)	98 (17)
O(22)	1116	2779	956 (30)	104 (18)
N(21)	925	4088	919 (30)	108 (25)
C(21)	2204	5595	843 (30)	51 (20)
C(22)	2102	4769	871 (30)	38 (17)
C(23)	2398	4174	883 (30)	42 (18)
C(24)	2295	3348	911 (30)	37 (18)
C(25)	1897	3118	928 (30)	71 (21)
C(26)	1601	3713	916 (30)	60 (20)
C(27)	1704	4539	887 (30)	52 (20)
C(28)	1408	5134	875 (30)	51 (18)
C(29)	1510	5960	847 (30)	39 (18)
C(30)	1908	6190	831 (30)	58 (21)
C(31)	1010	4904	892 (30)	100 (26)
C(32)	1203	3483	932 (30)	113 (29)
C(33)	510	3848	936 (30)	103 (32)
C(34)	321 (24)	3673 (50)	–796 (99)	100 (29)

Table 4. Structure (3): atomic coordinates ( $\times 10^4$ ) and equivalent isotropic temperature factors ( $\text{Å}^2 \times 10^3$ )

	x	y	z	$U_{eq}$
O(1)	–3827 (1)	390 (3)	1270 (1)	62 (11)
O(2)	–2430 (2)	5465 (3)	306 (1)	58 (11)
N(1)	–3121 (2)	2904 (3)	767 (1)	44 (11)
C(1)	–804 (2)	–979 (4)	411 (2)	40 (2)
C(2)	–793 (2)	756 (4)	212 (2)	38 (2)
C(3)	–5 (2)	1725 (4)	–208 (2)	40 (2)
C(4)	–25 (2)	3361 (4)	–421 (2)	45 (2)
C(5)	–799 (2)	4078 (4)	–210 (2)	47 (2)
C(6)	–1571 (2)	3178 (4)	206 (2)	42 (2)
C(7)	–1574 (2)	1478 (4)	407 (2)	39 (2)
C(8)	–2350 (2)	492 (4)	787 (2)	41 (2)
C(9)	–2336 (2)	–1172 (4)	960 (2)	48 (2)
C(10)	–1575 (2)	–1880 (4)	778 (2)	48 (2)
C(11)	–3150 (2)	1194 (4)	964 (2)	46 (2)
C(12)	–2381 (2)	3962 (4)	420 (2)	44 (2)
C(13)	–3909 (2)	3603 (5)	933 (2)	52 (2)
C(14)	–4545 (2)	4264 (5)	1593 (2)	65 (2)
C(15)	–5318 (3)	4816 (6)	1754 (3)	92 (3)
C(16)	–5428 (3)	4738 (7)	1270 (4)	101 (3)
C(17)	–4778 (3)	4108 (6)	614 (3)	85 (3)
C(18)	–3998 (3)	3523 (5)	433 (2)	60 (2)
C(19)	–3271 (3)	2864 (6)	–285 (2)	80 (3)
C(20)	–4402 (3)	4383 (8)	2110 (2)	99 (3)
O(21)	1632 (2)	893 (4)	6493 (1)	80 (2)
O(22)	1842 (2)	3425 (4)	8003 (1)	80 (2)
N(21)	1767 (2)	2038 (4)	7248 (1)	52 (2)
C(21)	4478 (2)	4092 (4)	4881 (2)	42 (2)
C(22)	4170 (2)	4314 (4)	5568 (2)	40 (2)
C(23)	4674 (2)	5215 (4)	5702 (2)	43 (2)
C(24)	4338 (2)	5379 (5)	6381 (2)	55 (2)
C(25)	3526 (2)	4729 (5)	6928 (2)	58 (2)
C(26)	3035 (2)	3834 (4)	6814 (2)	48 (2)
C(27)	3353 (2)	3615 (4)	6130 (2)	42 (2)
C(28)	2854 (2)	2677 (4)	6008 (2)	46 (2)
C(29)	3150 (2)	2520 (5)	5346 (2)	51 (2)
C(30)	3944 (2)	3227 (4)	4794 (2)	47 (2)
C(31)	2045 (2)	1807 (5)	6580 (2)	54 (2)
C(32)	2184 (2)	3131 (5)	7399 (2)	55 (2)
C(33)	979 (2)	1145 (5)	7808 (2)	55 (2)
C(34)	178 (2)	1842 (6)	8115 (2)	68 (2)
C(35)	–566 (3)	859 (7)	8627 (2)	85 (3)
C(36)	–473 (3)	–739 (7)	8803 (2)	96 (3)
C(37)	330 (3)	–1384 (7)	8504 (2)	89 (3)
C(38)	1080 (3)	–490 (5)	7995 (2)	71 (2)
C(39)	1966 (3)	–1219 (7)	7662 (3)	119 (4)
C(40)	101 (3)	3600 (8)	7915 (3)	105 (3)

Table 5. Structure (3): bond lengths (Å)

O(1)–C(11)	1.216 (4)	O(2)–C(12)	1.221 (4)
N(1)–C(11)	1.406 (4)	N(1)–C(12)	1.405 (4)
N(1)–C(13)	1.448 (5)	C(1)–C(2)	1.434 (5)
C(1)–C(3')	1.465 (5)	C(1)–C(10)	1.377 (4)
C(2)–C(3)	1.428 (4)	C(2)–C(7)	1.415 (5)
C(3)–C(4)	1.390 (5)	C(4)–C(5)	1.388 (6)
C(5)–C(6)	1.378 (4)	C(6)–C(7)	1.413 (5)
C(6)–C(12)	1.470 (5)	C(7)–C(8)	1.417 (4)
C(8)–C(9)	1.371 (5)	C(8)–C(11)	1.461 (6)
C(9)–C(10)	1.387 (6)	C(13)–C(14)	1.396 (5)
C(13)–C(18)	1.380 (8)	C(14)–C(15)	1.388 (8)
C(14)–C(20)	1.502 (9)	C(15)–C(16)	1.371 (14)
C(16)–C(17)	1.386 (8)	C(17)–C(18)	1.390 (9)
C(18)–C(19)	1.515 (5)	O(21)–C(31)	1.209 (6)
O(22)–C(32)	1.228 (5)	N(21)–C(31)	1.408 (5)
N(21)–C(33)	1.400 (6)	N(21)–C(33)	1.455 (4)
C(21)–C(22)	1.432 (5)	C(21)–C(23')	1.463 (4)
C(21)–C(30)	1.389 (6)	C(22)–C(23)	1.430 (6)
C(22)–C(27)	1.419 (4)	C(23)–C(24)	1.390 (6)
C(24)–C(25)	1.390 (4)	C(25)–C(26)	1.372 (7)
C(26)–C(27)	1.417 (5)	C(26)–C(32)	1.470 (4)
C(27)–C(28)	1.416 (6)	C(28)–C(29)	1.376 (6)
C(28)–C(31)	1.473 (4)	C(29)–C(30)	1.392 (4)
C(33)–C(34)	1.367 (6)	C(33)–C(38)	1.413 (6)
C(34)–C(35)	1.418 (5)	C(34)–C(40)	1.498 (8)
C(35)–C(36)	1.371 (8)	C(36)–C(37)	1.357 (8)
C(37)–C(38)	1.386 (6)	C(38)–C(39)	1.502 (8)

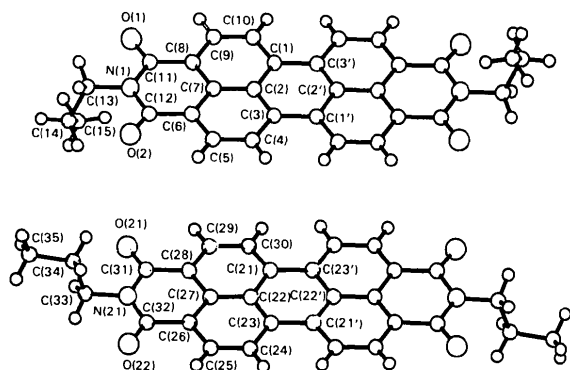


Fig. 1. Structure of molecules (I) (top) and (II) (bottom) of pigment (1).

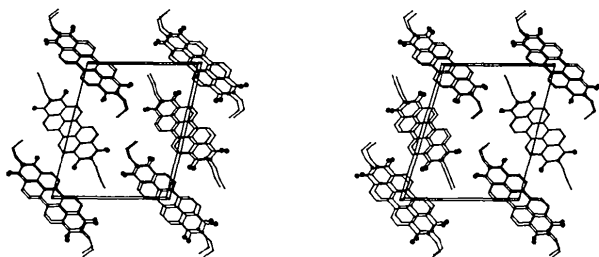


Fig. 2. Stereo packing plot projected down *c* for (1). The *b* axis is horizontal, left to right; the *a* axis is vertical, top to bottom.

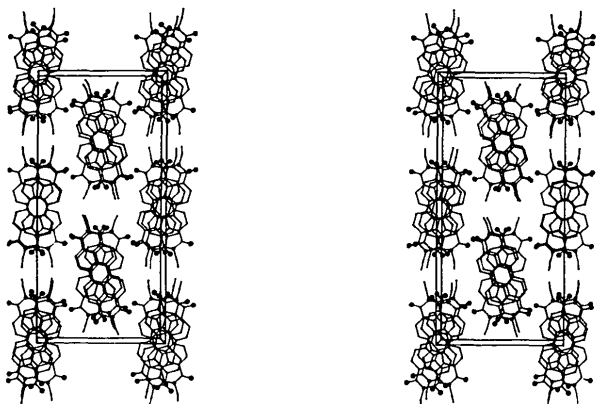


Fig. 3. Stereo packing plot projected down *c* for (2). The *b* axis is horizontal, left to right; the *a* axis is vertical, top to bottom.

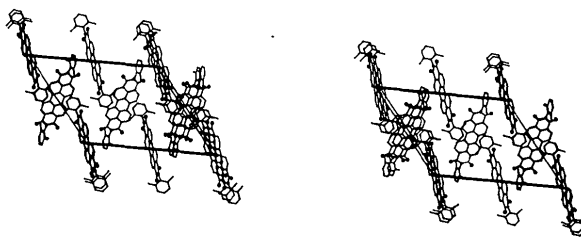


Fig. 4. Stereo packing plot projected down *b* for (3). The *c* axis is horizontal, left to right; the *a* axis is vertical, top to bottom.

The single molecules of all structures show a flat perylenetetracarboxylic diimide part with bent side chains.

Neighbouring molecules of (1) and (2) are arranged in stacks (Figs. 2 and 3) with a distance between the flat parts of from 3.408–3.443 Å (with e.s.d.'s of 0.010–0.039 Å).

In structure (1) the stacks of molecules (I) and (II) make an angle of 21.1 (6)°. The stacks of (2) are arranged along the *c* direction. In each stack of (2) the molecules are alternately oriented. The nearest neighbours in (2) are rotated by 31.0 (25)°, where the nearest-but-one neighbours have the same orientation.

Owing to the nearly perpendicular [80.6 (7) and 82.9 (7)°] arrangement of the phenyl rings to the perylene-imide ring system of structure (3), no stacks could be formed. Therefore the molecular packing (Fig. 4) differs from that of the other perylenetetracarboxylic diimide pigments investigated.

Correlations between the colours of the crystals and the crystal packing are discussed elsewhere in detail (Graser & Hädicke, 1980, 1984).

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