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## Structure of Dibenzo[*def,i*]naphtho[1,8,7-*vw*x]pyranthrene

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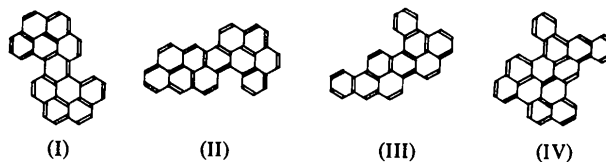
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**Abstract.**  $C_{42}H_{20}$ ,  $M_r = 524.6$ , orthorhombic,  $Pn2_1a$ ,  $a = 22.52$  (1),  $b = 21.313$  (7),  $c = 4.950$  (4) Å,  $V = 2375.9$  (8) Å<sup>3</sup>,  $Z = 4$ ,  $D_m = 1.46$ ,  $D_x = 1.467$  g cm<sup>-3</sup>,  $\lambda(\text{Cu K}\alpha) = 1.5418$  Å,  $\mu = 6.52$  cm<sup>-1</sup>,  $F(000) = 1088$ ,  $T = 298$  K. Final  $R = 0.044$  for 1442 independent reflections. The molecule is largely distorted from a planar structure owing to the steric repulsion between the intramolecular overcrowded atoms. The deviations of the atoms from the mean molecular plane range from 1.07 (1) to -0.74 (1) Å. Molecules are stacked face-to-face to make a columnar structure along the  $c$  axis. The distance between the mean molecular planes is 3.60 Å.

**Introduction.** In a serial study of the molecular distortion due to 1,7-interaction, the crystal structures of three compounds have already been determined: (I) diphenanthro[5,4,3-*abcd*:5',4',3'-*ijklm*]perylene (DPP) (Oonishi, Fujisawa, Aoki & Danno, 1978); (II) anthra[2,1,9,8-*hijkl*]benzo[*de*]naphtho[2,1,8,7-*stuv*]pentacene (1,11-BisoVEB) (Fujisawa, Oonishi, Aoki, Ohashi & Sasada, 1982); and (III) dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene (VEB) (Oonishi, Fujisawa, Aoki, Ohashi & Sasada, 1986). Recently the title compound, (IV), has been prepared from the condensation of 13*H*-dibenz[*a,de*]anthracen-13-one and 7*H*-benzo[*hi*]chrysen-7-one with zinc dust in the

presence of ZnCl<sub>2</sub> and NaCl. In order to compare its structure with those of the compounds mentioned above, a crystal structure analysis has been carried out.



**Experimental.** Reddish-brown needle-like crystals from *o*-dichlorobenzene solution;  $D_m$  by flotation in ZnCl<sub>2</sub> solution; systematic absences:  $0kl$ ,  $k+l = 2n+1$ ,  $hk0$ ,  $h = 2n+1$ ; crystal dimensions 0.6 × 0.2 × 0.1 mm; Rigaku AFC-6 diffractometer; graphite monochromator; cell parameters refined by least-squares method on the basis of 25 independent  $2\theta$  values;  $41 < 2\theta < 57^\circ$ , intensity measurement performed up to  $2\theta = 125^\circ$ ; range of  $hkl$  0 to 25, 0 to 24 and 0 to 5;  $\omega-2\theta$  scan, scan speed  $4^\circ \text{ min}^{-1}(\theta)$ , scan width  $(1.50 + 0.45 \tan \theta)^\circ$ ; background 5 s before and after each scan; three standard reflections monitored every 100 reflections, no significant variation in intensities; 1878 reflections measured, 1442 with  $|F_o| > 3\sigma(|F_o|)$  considered observed and used for structure determination; corrections for Lorentz and polarization,

Table 1. Final atomic coordinates ( $\times 10^5$ ) and equivalent isotropic thermal parameters,  $B_{eq}(\text{\AA}^2) (\times 10)$ 

$$B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	$B_{eq}$
C(1)	8480 (3)	6735 (2)	-1550 (11)	54 (2)
C(2)	9028 (2)	6964 (2)	-892 (12)	55 (2)
C(3)	9365 (3)	6683 (2)	1036 (11)	52 (2)
C(4)	9154 (2)	6159 (2)	2416 (12)	47 (1)
C(5)	9477 (2)	5874 (2)	4575 (11)	47 (1)
C(6)	9290 (2)	5343 (2)	5743 (10)	43 (1)
C(7)	8745 (2)	5040 (2)	4978 (10)	40 (1)
C(8)	8554 (2)	4475 (2)	6136 (9)	38 (1)
C(9)	8950 (2)	4049 (2)	7606 (11)	43 (1)
C(10)	9573 (2)	4041 (2)	7070 (12)	50 (1)
C(11)	9948 (3)	3666 (2)	8558 (12)	53 (2)
C(12)	9729 (2)	3279 (3)	10527 (12)	54 (2)
C(13)	9129 (3)	3239 (3)	10915 (11)	53 (2)
C(14)	8726 (2)	3599 (2)	9409 (10)	41 (1)
C(15)	8081 (2)	3494 (2)	9534 (10)	38 (1)
C(16)	7832 (2)	3061 (2)	11200 (10)	44 (1)
C(17)	7222 (2)	2914 (2)	11132 (10)	43 (1)
C(18)	6976 (3)	2467 (2)	13009 (11)	50 (2)
C(19)	6385 (3)	2336 (2)	13025 (12)	56 (2)
C(20)	6013 (3)	2640 (3)	11165 (12)	58 (2)
C(21)	6225 (2)	3066 (3)	9365 (11)	52 (2)
C(22)	6846 (2)	3220 (2)	9322 (10)	40 (1)
C(23)	7093 (2)	3680 (2)	7475 (11)	41 (1)
C(24)	6740 (2)	3984 (2)	5540 (10)	40 (1)
C(25)	6956 (2)	4447 (2)	3914 (10)	38 (1)
C(26)	6588 (2)	4758 (2)	1817 (10)	41 (1)
C(27)	5998 (2)	4581 (3)	1372 (11)	46 (1)
C(28)	5653 (2)	4861 (3)	-586 (11)	52 (2)
C(29)	5884 (2)	5329 (3)	-2128 (11)	54 (2)
C(30)	6470 (2)	5541 (2)	-1722 (10)	44 (1)
C(31)	6726 (2)	6037 (2)	-3328 (11)	51 (2)
C(32)	7279 (3)	6231 (2)	-2866 (11)	52 (2)
C(33)	7654 (2)	5958 (2)	-807 (10)	42 (1)
C(34)	8234 (2)	6203 (2)	-253 (10)	43 (1)
C(35)	8582 (2)	5910 (2)	1740 (10)	43 (1)
C(36)	8374 (2)	5358 (2)	3145 (10)	38 (1)
C(37)	7940 (2)	4302 (2)	5928 (10)	38 (1)
C(38)	7707 (2)	3813 (2)	7617 (10)	38 (1)
C(39)	7569 (2)	4636 (2)	4172 (9)	35 (1)
C(40)	7790 (2)	5141 (2)	2617 (10)	39 (1)
C(41)	7427 (2)	5456 (2)	641 (9)	39 (1)
C(42)	6829 (2)	5247 (2)	245 (10)	39 (1)

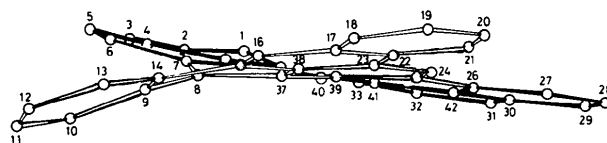
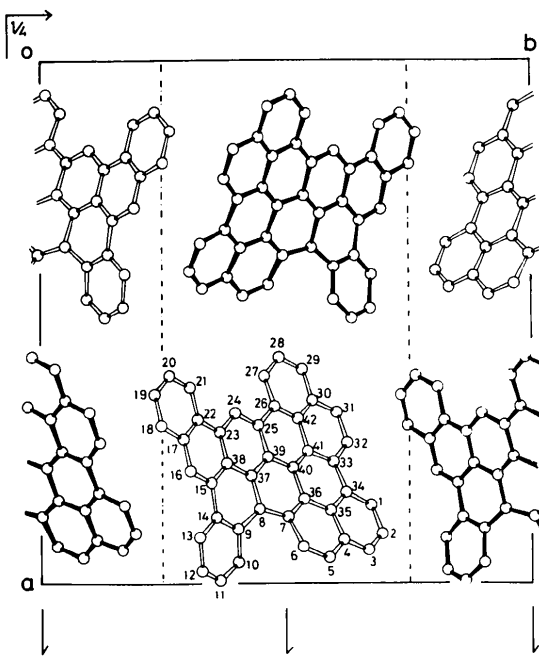


Fig. 2. Perspective drawing of the molecule.

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ) with their standard deviations

C(1)–C(2)	1.366 (8)	C(21)–C(22)	1.434 (8)
C(1)–C(34)	1.414 (8)	C(22)–C(23)	1.451 (7)
C(2)–C(3)	1.358 (8)	C(23)–C(24)	1.403 (7)
C(3)–C(4)	1.390 (8)	C(23)–C(38)	1.411 (7)
C(4)–C(5)	1.427 (8)	C(24)–C(25)	1.363 (7)
C(4)–C(35)	1.432 (8)	C(25)–C(26)	1.483 (7)
C(5)–C(6)	1.338 (7)	C(25)–C(39)	1.443 (7)
C(6)–C(7)	1.436 (7)	C(26)–C(27)	1.396 (7)
C(7)–C(8)	1.402 (7)	C(26)–C(42)	1.409 (7)
C(7)–C(36)	1.407 (7)	C(27)–C(28)	1.376 (8)
C(8)–C(9)	1.464 (7)	C(28)–C(29)	1.359 (8)
C(8)–C(37)	1.433 (7)	C(29)–C(30)	1.407 (8)
C(9)–C(10)	1.427 (8)	C(30)–C(31)	1.443 (7)
C(9)–C(14)	1.403 (7)	C(30)–C(42)	1.412 (7)
C(10)–C(11)	1.374 (8)	C(31)–C(32)	1.331 (8)
C(11)–C(12)	1.368 (9)	C(32)–C(33)	1.445 (8)
C(12)–C(13)	1.367 (8)	C(33)–C(34)	1.432 (7)
C(13)–C(14)	1.402 (8)	C(33)–C(41)	1.385 (7)
C(14)–C(15)	1.470 (7)	C(34)–C(35)	1.406 (7)
C(15)–C(16)	1.359 (7)	C(35)–C(36)	1.443 (7)
C(15)–C(38)	1.438 (7)	C(36)–C(40)	1.416 (7)
C(16)–C(17)	1.408 (8)	C(37)–C(38)	1.434 (7)
C(17)–C(18)	1.439 (8)	C(37)–C(39)	1.400 (7)
C(17)–C(22)	1.393 (7)	C(39)–C(40)	1.413 (7)
C(18)–C(19)	1.359 (8)	C(40)–C(41)	1.440 (7)
C(19)–C(20)	1.402 (9)	C(41)–C(42)	1.430 (7)
C(20)–C(21)	1.358 (8)		
C(2)–C(1)–C(34)	122.2 (6)	C(24)–C(25)–C(39)	119.3 (5)
C(1)–C(2)–C(3)	120.8 (6)	C(26)–C(25)–C(39)	118.1 (5)
C(2)–C(3)–C(4)	120.7 (6)	C(25)–C(26)–C(42)	121.3 (5)
C(3)–C(4)–C(5)	122.5 (6)	C(25)–C(26)–C(42)	120.1 (5)
C(3)–C(4)–C(35)	119.3 (6)	C(27)–C(26)–C(42)	118.6 (5)
C(5)–C(4)–C(35)	118.2 (5)	C(26)–C(27)–C(28)	122.0 (5)
C(4)–C(5)–C(6)	121.6 (5)	C(27)–C(28)–C(29)	119.8 (6)
C(5)–C(6)–C(7)	122.3 (5)	C(28)–C(29)–C(30)	120.9 (6)
C(6)–C(7)–C(8)	122.7 (5)	C(29)–C(30)–C(31)	122.1 (5)
C(6)–C(7)–C(36)	117.4 (5)	C(29)–C(30)–C(42)	119.4 (5)
C(8)–C(7)–C(36)	119.8 (5)	C(31)–C(30)–C(42)	118.5 (5)
C(7)–C(8)–C(9)	123.4 (5)	C(30)–C(31)–C(32)	120.4 (6)
C(7)–C(8)–C(37)	119.1 (5)	C(31)–C(32)–C(33)	122.8 (6)
C(9)–C(8)–C(37)	117.5 (5)	C(32)–C(33)–C(34)	121.3 (5)
C(8)–C(9)–C(10)	120.8 (5)	C(32)–C(33)–C(41)	117.5 (5)
C(8)–C(9)–C(14)	121.5 (5)	C(34)–C(33)–C(41)	121.3 (5)
C(10)–C(9)–C(14)	117.5 (5)	C(1)–C(34)–C(35)	124.2 (5)
C(9)–C(10)–C(11)	120.7 (6)	C(1)–C(34)–C(35)	117.2 (5)
C(10)–C(11)–C(12)	120.7 (6)	C(33)–C(34)–C(35)	118.6 (5)
C(11)–C(12)–C(13)	119.6 (6)	C(4)–C(35)–C(34)	119.9 (5)
C(12)–C(13)–C(14)	121.9 (6)	C(4)–C(35)–C(36)	118.8 (5)
C(9)–C(14)–C(13)	118.8 (5)	C(34)–C(35)–C(36)	121.3 (5)
C(9)–C(14)–C(15)	119.0 (5)	C(7)–C(36)–C(35)	120.7 (5)
C(13)–C(14)–C(15)	122.1 (5)	C(7)–C(36)–C(40)	120.7 (5)
C(14)–C(15)–C(16)	122.4 (5)	C(35)–C(36)–C(40)	118.6 (5)
C(14)–C(15)–C(38)	118.5 (5)	C(8)–C(37)–C(38)	119.8 (5)
C(16)–C(15)–C(38)	118.8 (5)	C(8)–C(37)–C(39)	119.2 (5)
C(15)–C(16)–C(17)	122.5 (5)	C(38)–C(37)–C(39)	120.9 (5)
C(16)–C(17)–C(18)	120.3 (5)	C(15)–C(38)–C(23)	120.6 (5)
C(16)–C(17)–C(22)	120.1 (5)	C(15)–C(38)–C(37)	121.0 (5)
C(18)–C(17)–C(22)	119.5 (5)	C(23)–C(38)–C(37)	118.3 (5)
C(17)–C(18)–C(19)	121.0 (6)	C(25)–C(39)–C(37)	118.9 (5)
C(18)–C(19)–C(20)	119.0 (6)	C(25)–C(39)–C(40)	120.1 (5)
C(19)–C(20)–C(21)	122.0 (6)	C(37)–C(39)–C(40)	121.0 (5)
C(20)–C(21)–C(22)	120.4 (6)	C(36)–C(40)–C(39)	118.4 (5)
C(17)–C(22)–C(21)	118.2 (5)	C(36)–C(40)–C(41)	119.9 (5)
C(17)–C(22)–C(23)	119.3 (5)	C(39)–C(40)–C(41)	121.6 (5)
C(21)–C(22)–C(23)	122.5 (5)	C(33)–C(41)–C(40)	120.1 (5)
C(22)–C(23)–C(24)	121.6 (5)	C(33)–C(41)–C(42)	121.1 (5)
C(22)–C(23)–C(38)	118.7 (5)	C(40)–C(41)–C(42)	118.8 (5)
C(24)–C(23)–C(38)	119.7 (5)	C(26)–C(42)–C(30)	119.2 (5)
C(23)–C(24)–C(25)	122.4 (5)	C(26)–C(42)–C(41)	121.1 (5)
C(24)–C(25)–C(26)	122.6 (5)	C(30)–C(42)–C(41)	119.7 (5)

Fig. 1. A projection of the crystal structure along the *c* axis and the numbering scheme.

absorption ignored; direct method (*MULTAN78*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and subsequent difference Fourier calculation; block-diagonal least squares (*HBL5*; Ohashi, 1975) with anisotropic thermal parameters for all non-H atoms; H atoms derived geometrically (C—H 1.08 Å) and refined;  $\sum w(|F_o| - |F_c|)^2$  minimized with  $w = [\sigma^2(F_o) + (0.03 F)^2]^{-1}$ ; max.  $(\Delta/\sigma)$  0.5; final  $R = 0.044$ ;  $\Delta\rho$  excursions in final difference map  $0.3 \text{ e } \text{Å}^{-3}$ ; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); calculation carried out on HITAC M-280 computer at the Computer Center of the University of Tokyo.

**Discussion.** The final atomic parameters for non-H atoms are given in Table 1.\* A projection of the structure along the *c* axis with the numbering scheme is given in Fig. 1 and a perspective drawing of the molecule is shown in Fig. 2. Bond distances and angles are listed in Table 2. The molecular structure is distorted to a large extent from a planar conformation due to steric repulsions between the intramolecular overcrowded hydrogen atoms; particularly H(C6) and H(C10). The repulsion is released mainly by the enlargement of the C(7)—C(8)—C(9) angle and distortion from the planar conformation. The degree of

\* Lists of structure factors, anisotropic thermal parameters for non-H atoms, and positional and thermal parameters for H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 43021 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

distortion was defined as the torsion angle around the pseudo-bond C(7)···C(9), C(6)—C(7)···C(9)—C(10) (Fujisawa, Oonishi, Aoki, Ohashi & Sasada, 1982). The values of C(7)—C(8)—C(9) and the torsion angle are  $123.4(5)$  and  $38.2(7)^\circ$ , respectively. These are comparable to those of VEB:  $124(1)$  and  $37(1)^\circ$ , but considerably different from those of the *A* molecule of 1,11-BisoVEB:  $128.7$  and  $30.1^\circ$ . The dihedral angles C(6)—C(7)—C(8)—C(9) and C(7)—C(8)—C(9)—C(10) are  $18.2$  and  $25.4^\circ$ , respectively. The deviations of the atoms from the mean molecular plane range from  $1.07(1)$  Å for C(11) to  $-0.74(1)$  Å for C(5).

The molecules are stacked face-to-face to make a columnar structure along the *c* axis by van der Waals forces. The distance between the mean molecular planes is  $3.60(1)$  Å. There is no unusual short contact between the columns.

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## 8-Methylbenz[*a*]anthracene

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**Abstract.**  $\text{C}_{19}\text{H}_{14}$ ,  $M_r = 242.3$ , monoclinic,  $P2/a$ ,  $a = 48.516(8)$ ,  $b = 6.527(3)$ ,  $c = 8.226(2)$  Å,  $\beta = 92.15(2)^\circ$ ,  $V = 2603.0 \text{ Å}^3$ ,  $Z = 8$ ,  $D_m = 1.22(1)$  (NaI

flotation),  $D_x = 1.237 \text{ g cm}^{-3}$ ,  $\lambda(\text{Cu K}\alpha) = 1.5418 \text{ Å}$ ,  $\mu = 5.6 \text{ cm}^{-1}$ ,  $F(000) = 1024$ ,  $T = 298 \text{ K}$ , final  $R = 0.051$  for 2343 observed reflections. The two molecules in the asymmetric unit are almost planar with inclinations of  $5.1(3)$  and  $2.4(3)^\circ$  between the outermost rings *A/D*. At the bay region the beach bond

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