

Fig. 2. Projection onto the plane of B(6), B(4), B(2), B(3).

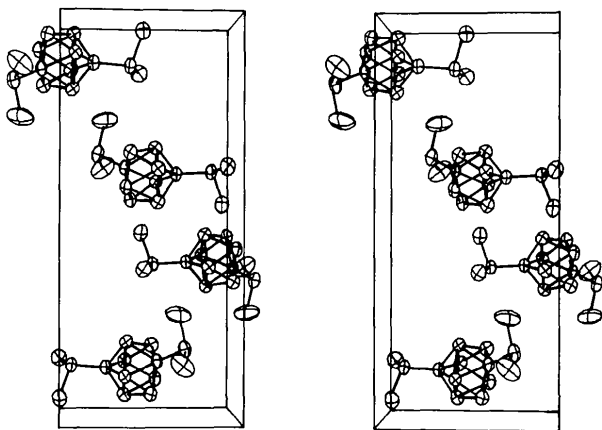


Fig. 3. Stereoscopic drawing (Johnson, 1965) of the contents of one unit cell.

opposite triangular faces is $1.4(3)^\circ$, and those between adjacent rectangular faces $62.9(3)$, $58.6(3)$ and $58.5(3)^\circ$. The bond angles within the cage are similar to those that would be expected for idealized D_{3h} symmetry and are in good agreement with those given by Guggenberger (1968).

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Structure of Flavanthrene*

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Abstract. $C_{28}H_{14}N_2$, monoclinic, $P2_1/a$, $a = 16.179(2)$, $b = 3.7996(2)$, $c = 15.818(1)$ Å, $\beta = 119.192(6)^\circ$, $U = 848.87(13)$ Å³, $Z = 2$, $D_m = 1.47$

There are no significant intermolecular contacts. The shortest nonbonded distances, excluding hydrogens, are $3.743(8)$ Å between S(1) and S(2) related by $x, y, z \rightarrow x, y - 1, z$; and $3.75(1)$ Å between B(9) and C(3) related by $x, y, z \rightarrow \frac{1}{2} + x, \frac{1}{2} - y, -z$.

A projection onto the plane of B(6), B(4), B(2), B(3) is shown in Fig. 2 and a stereoview is shown in Fig. 3.

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* Alternative name: 5,13-diazapyranthrene.

(by flotation in carbon tetrachloride/*n*-hexane), $D_x = 1.48$ Mg m⁻³, $M_r = 378.43$, $\mu(\text{Cu } K\alpha) = 0.69$ mm⁻¹. The final R is 0.041 for 1445 independent observed amplitudes. The flavanthrene molecule is planar, and the interplanar distance is $3.4711(5)$ Å. The propor-

tion of overlapped area of the molecular plane is about 54%.

Introduction. Flavanthrene was obtained by the reduction of flavantrone according to the reported procedure (Aoki, 1968). Crystals suitable for crystallographic analysis were grown by sublimation *in vacuo* at 543 K; thick reddish-brown plates with (001) developed were obtained.

Intensity data were collected on a Rigaku four-circle diffractometer with graphite-monochromatized Cu $K\alpha$ radiation, employing the θ - 2θ scan technique. A crystal of dimensions $0.4 \times 0.4 \times 0.09$ mm was used for the data collection up to $2\theta = 155^\circ$. Of 2031 reflections, 1445 independent reflections with $|F| > 3\sigma(F)$ were obtained, and used in the structure analysis. Lorentz-polarization and absorption corrections were applied. The cell dimensions were determined by a least-squares calculation on the basis of 45 2θ values ($36^\circ < 2\theta < 56^\circ$) measured on the diffractometer.

The structure was solved from three-dimensional Patterson maps and refined by the block-diagonal least-squares method. The weighting scheme $w = [\sigma_c^2 + (0.015|F|)^2]^{-1}$ was employed. H-atom positions were derived from difference Fourier maps, and included in the refinement with isotropic temperature factors. The final R and R_w values were 0.041 and 0.065, respectively. The scattering factors and anomalous-scattering corrections for non-H atoms were taken from *International Tables for X-ray*

Table 1. *Final positional parameters* ($\times 10^4$ for non-H atoms; $\times 10^3$ for H atoms) and isotropic thermal parameters

	x	y	z	B_{eq}^*/B (\AA^2)
N	1692 (1)	2208 (3)	753 (1)	2.54 (3)
C(1)	1545 (1)	1071 (3)	1489 (1)	2.37 (3)
C(2)	2312 (1)	1333 (3)	2469 (1)	2.50 (3)
C(3)	3198 (1)	2762 (3)	2683 (1)	2.90 (4)
C(4)	3919 (1)	2926 (4)	3618 (1)	3.39 (4)
C(5)	3788 (1)	1707 (4)	4383 (1)	3.48 (4)
C(6)	2935 (1)	336 (4)	4199 (1)	3.15 (4)
C(7)	2170 (1)	111 (3)	3241 (1)	2.63 (3)
C(8)	1281 (1)	-1313 (3)	3042 (1)	2.78 (3)
C(9)	539 (1)	-1552 (3)	2114 (1)	2.49 (3)
C(10)	-381 (1)	-2968 (3)	1870 (1)	2.77 (3)
C(11)	-1101 (1)	-3168 (3)	954 (1)	2.77 (4)
C(12)	-980 (1)	-1976 (3)	151 (1)	2.37 (4)
C(13)	-74 (1)	-584 (3)	376 (1)	2.26 (4)
C(14)	677 (1)	-358 (3)	1332 (1)	2.30 (4)
H(C3)	327 (1)	368 (4)	215 (1)	4.6 (3)
H(C4)	453 (1)	385 (5)	376 (1)	5.1 (4)
H(C5)	431 (1)	176 (4)	507 (1)	4.8 (4)
H(C6)	282 (1)	-53 (4)	474 (1)	4.4 (3)
H(C8)	120 (1)	-207 (4)	361 (1)	3.8 (3)
H(C10)	-50 (1)	-377 (4)	240 (1)	3.9 (3)
H(C11)	-172 (1)	-423 (4)	81 (1)	4.0 (3)

* For non-H atoms $B_{eq} = \frac{1}{3} \sum_i \sum_j a_i \cdot a_j \beta_{ij}$.

Crystallography (1974). For H the values given by Stewart, Davidson & Simpson (1965) were used. The final atomic coordinates are listed in Table 1.*

Discussion. The molecular structure and dimensions of the title compound are presented in Fig. 1. The flavanthrene molecule sits on a center of symmetry. All the C-C bond distances are within the range 1.347 (1)–1.450 (2) \AA . Fig. 2 shows deviations of atoms from the least-squares plane defined by all the non-H atoms. The flavanthrene molecule is planar, and deviations from the plane are less than 0.015 \AA except for the C(3) atom, which deviates from the plane by 0.023 (1) \AA . This is caused by a non-bonded interaction between N and HC(3) atoms at a distance of 2.49 (1) \AA .

A stereoscopic view of the crystal packing is given in Fig. 3. Flavanthrene forms a 'roof-top' type of stacking (Stadler, 1964). The mode of superposition of flavanthrene molecules is shown in Fig. 4, which is a projection along the normal to the molecular plane. This feature is similar to that of a graphite crystal, but there is a significant lateral shift of the C atoms compared to the graphite-like superposition. The interplanar spacing between molecules is 3.4711 (5) \AA , which is in the normal range 3.38–3.52 \AA found in the large aromatic hydrocarbons (Stadler, 1964), and comparable to 3.44 \AA in flavantrone (Stadler, 1953)

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36384 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

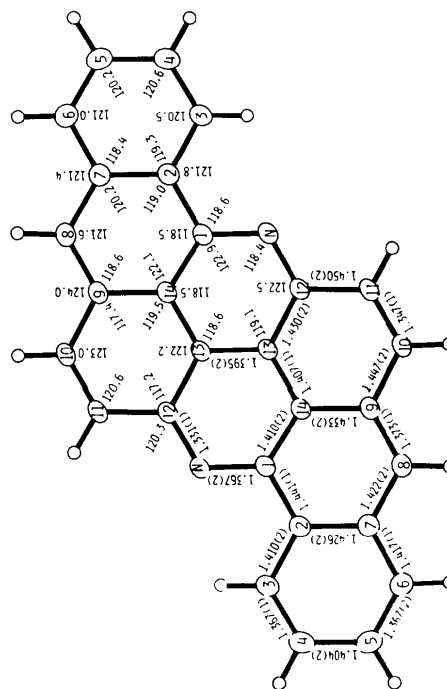


Fig. 1. Bond distances (\AA) and angles ($^\circ$) with the atom-numbering scheme. E.s.d.'s for angles are all 0.1 $^\circ$. The thermal ellipsoids are the 30% probability surfaces.

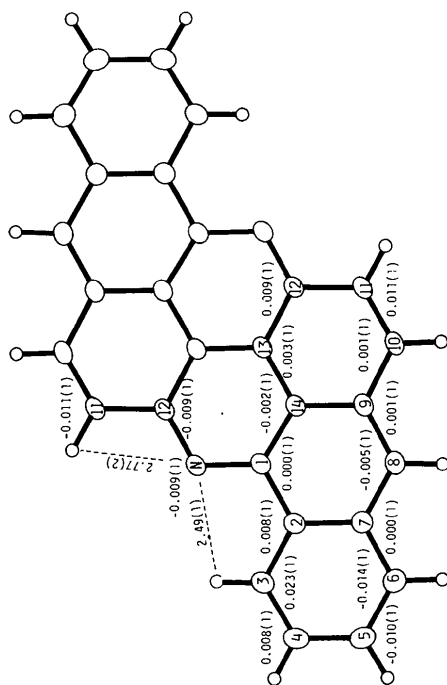


Fig. 2. Deviations of non-H atoms from the least-squares plane and selected interatomic distances (Å) within the molecule.

and 3.44 and 3.46 Å in pyranthrone (Maitland & Stadler, 1966; Stadler 1964). The proportion of overlapped area of the molecular plane, which is illustrated by the shaded area in Fig. 4, is 54% for flavanthrene. This ratio is smaller than those of the related quinones, flavanthrene (68%) and pyranthrone (68, 66%) (Stadler, 1964).

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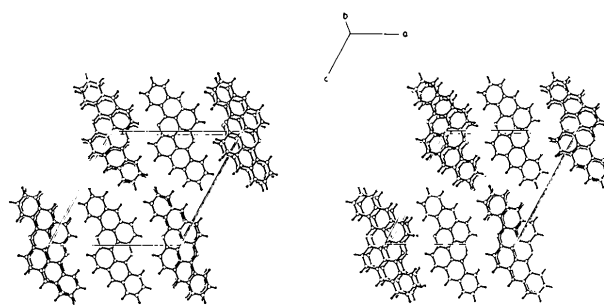


Fig. 3. Stereoscopic drawing of the crystal packing viewed along the *b* axis.

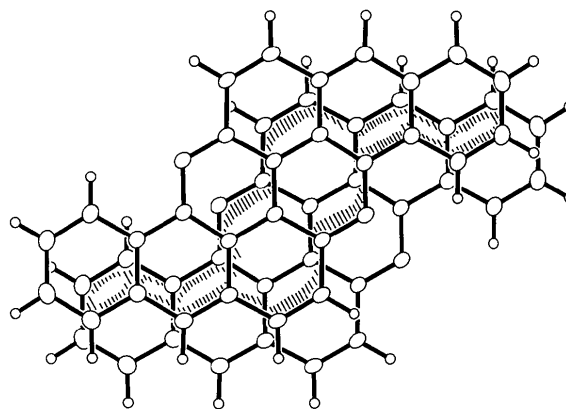


Fig. 4. Stacking of two neighboring flavanthrene molecules viewed along the normal to the molecular plane. The area enclosed by shading shows the overlapped part of the molecular plane.

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