Fig. 2. Packing diagram projected down **b**. H atoms are omitted for clarity.

Discussion. The geometry at the N atom is approximately planar, with angles at N of 121·6, 121·0 and 117·2° and deviations Si(1) 0·01, N(1) −0·03, Si(2) 0·01, C(41) 0·01 Å from the mean plane of the four atoms. This may be attributed to the familiar $d\pi$–$p\pi$ bonding in Si—N compounds, typified by trisilylamine (Beagley & Conrad, 1970). The N—Si distances are significantly different [1·732 (4) and 1·712 (4) Å respectively for N(1)—Si(1) and N(1)—Si(2)]. This may be due to the greater electronegativity of the SiF$_2$ group inducing more $d\pi$–$p\pi$ bonding between N(1) and Si(2). An alternative explanation, however, is a change in

covalent radii on changing the electronegativities of the substituents; thus the Si—H length (determined by microwave spectroscopy) changes from 1·485 ± 0·01 Å in SiH$_3$F (Kewley, McKinney & Robiette, 1970) to 1·455 ± 0·01 Å in SiHF$_3$ (Heath, Thomas & Sheridan, 1954), and there are clearly no possible π interactions for the Si—H bond. The mesitylene ring cannot be involved in π interactions with the Si—N—Si system as it is approximately perpendicular to it [torsion angles Si(1)—N(1)—C(41)—C(42) −82·1°, Si(2)—N(1)—C(41)—C(42) 92·9°].

The only short non-bonded contact is C(56)$\cdots$F(3) 3·06 Å (second atom at $\frac{1}{2} - x$, $-\frac{1}{2} + y$, z).

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Melitracene Hydrobromide: 9-(3-Dimethylaminopropylidene)-10,10-dimethyl-9,10-dihydroanthracene Hydrobromide

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Abstract. C$_{21}$H$_{26}$N$^+$·Br$^-$, $M_r = 372·36$, monoclinic, $P2_1/c$, $a = 17·680$ (2), $b = 10·3084$ (4), $c = 22·618$ (2) Å, $\beta = 107·92$ (1)°, $U = 3922$ (1) Å^3, $Z = 8$, $D_x = 1·25$ Mg m^{-3}, μ(Mo $K\alpha$) = 2·577 mm^{-1}. Melitracene is a tricyclic antidepressant. Its structure was refined to $R = 0·064$ for 2813 independent reflexions. The molecules are held together by salt bridges and van der Waals forces. The molecular conformation and other data of pharmacological interest are given.

Introduction. From this study of the crystal structure of melitracene and studies of other antidepressant drugs in progress, we have accumulated information about their conformations and charge distributions from which

conclusions may be drawn about the structure–activity relation.

A crystalline sample of melitracene hydrochloride was kindly provided by Abelló Laboratories (Madrid). The sample was transformed to the hydrobromide and recrystallized from water. A crystal ~0·3 × 0·3 × 0·4 mm was selected for the X-ray investigation. The intensities of all 6899 unique reflexions with $2 < \theta < 25°$ were measured at 295 K with monochromatic Mo $K\alpha$ radiation on a Philips PW 1100 diffractometer. An ω–2θ scan technique was used. There was no appreciable change in the periodically monitored standard reflexions. No correction for absorption was applied and 2813 data were accepted on the criterion $I > 2\sigma(I)$. Structure amplitudes were obtained after Lorentz and polarization corrections.

The positions of the heavy atoms were obtained from a Patterson map. All remaining non-hydrogen atoms were located from a difference synthesis. Scattering factors for neutral atoms were taken from *International Tables for X-ray Crystallography* (1974). The H atoms were set at their calculated positions. The structure was refined anisotropically by least squares. In order to prevent bias on ΔF vs F_o or sin θ/λ, weights were assigned as $w = 1/(a + b|F_o|)^2$ with coefficients calculated with *PESOS* (Martínez-Ripoll & Cano, 1975) to be $a = 4·57$, $b = -0·15$ for $F_o \leq 5$, $a = 3·21$, $b = 0·12$ for $5 < F_o < 15$, $a = 7·18$, $b = -0·16$ for $15 \leq F_o < 33$, $a = 2·34$, $b = -0·01$ for $33 \leq F_o < 50$, and $a = 0·71$, $b = 0·03$ for other data. Final refinement, with isotropic temperature factors for H atoms gave $R = 0·064$ and $R_w = (\sum w\Delta^2/\sum w|F_o|^2)^{1/2} = 0·066$. Table 1 shows the final coordinates of the non-hydrogen atoms.*

Discussion. The crystal structure is shown in projection along b in Fig. 1. The folding of the side chains is approximately parallel to a. Each molecule is involved in a salt bridge, as a result of proton transfer from BrH(1) and BrH(2) to N(1) and N(2), respectively, forming the hydrogen-bonded ion-pair $N^+H\cdots Br^-$ (Table 2). Other intermolecular interactions are due to van der Waals forces.

The geometrical features of the independent molecules are shown in Fig. 2. All phenyl rings have their usual geometry. Both central rings have a boat

Table 1. *The positional parameters* $(\times 10^4)$ *for non-hydrogen atoms*

E.s.d.'s are given in parentheses.

	x	y	z
Br(1)	5639 (1)	2924 (1)	2542 (1)
N(1)	5506 (5)	5088 (7)	1481 (4)
C(11)	8444 (7)	5167 (11)	1405 (5)
C(12)	8906 (8)	6216 (11)	1418 (5)
C(13)	9168 (7)	6523 (11)	924 (7)
C(14)	8968 (7)	5702 (11)	401 (5)
C(15)	8234 (6)	3728 (9)	−189 (4)
C(16)	7384 (7)	4047 (11)	−556 (5)
C(17)	8766 (8)	3894 (12)	−604 (5)
C(18)	8544 (6)	1287 (12)	−203 (5)
C(19)	8516 (7)	41 (12)	24 (6)
C(110)	8189 (8)	−203 (11)	485 (6)
C(111)	7908 (7)	791 (10)	748 (5)
C(112)	7945 (5)	2086 (9)	531 (4)
C(113)	8244 (5)	2339 (9)	51 (4)
C(114)	8484 (6)	4632 (9)	380 (4)
C(115)	8198 (6)	4358 (9)	883 (4)
C(116)	7701 (6)	3185 (9)	846 (5)
C(117)	7066 (6)	3131 (10)	1057 (5)
C(118)	6751 (7)	4158 (12)	1387 (6)
C(119)	5894 (7)	4403 (9)	1060 (5)
C(120)	4644 (7)	5315 (11)	1158 (6)
C(121)	5913 (7)	6324 (9)	1740 (4)
Br(2)	5672 (1)	−2363 (1)	88 (1)
N(2)	5590 (4)	−260 (6)	960 (3)
C(21)	7677 (6)	302 (8)	−1905 (4)
C(22)	8097 (7)	1416 (10)	−1959 (4)
C(23)	8884 (8)	1355 (11)	−1908 (5)
C(24)	9284 (6)	188 (11)	−1808 (4)
C(25)	9286 (5)	−2302 (9)	−1647 (4)
C(26)	9492 (6)	−2596 (10)	−940 (4)
C(27)	73 (6)	−2308 (12)	−1790 (5)
C(28)	8949 (7)	−4380 (11)	−2282 (5)
C(29)	8405 (9)	−5301 (11)	−2581 (5)
C(210)	7619 (7)	−5234 (11)	−2620 (5)
C(211)	7373 (7)	−4173 (10)	−2357 (5)
C(212)	7921 (6)	−3218 (8)	−2039 (4)
C(213)	8701 (6)	−3318 (9)	−2003 (4)
C(214)	8891 (6)	−961 (9)	−1761 (4)
C(215)	8093 (6)	−870 (8)	−1792 (4)
C(216)	7657 (5)	−2105 (9)	−1737 (4)
C(217)	7110 (5)	−2259 (8)	−1449 (4)
C(218)	6825 (6)	−1305 (9)	−1074 (4)
C(219)	5960 (6)	−959 (8)	−1387 (4)
C(220)	4731 (6)	−28 (10)	−1280 (5)
C(221)	6017 (7)	953 (10)	−699 (5)

* Lists of structure factors, thermal parameters and H atom positional parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34319 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
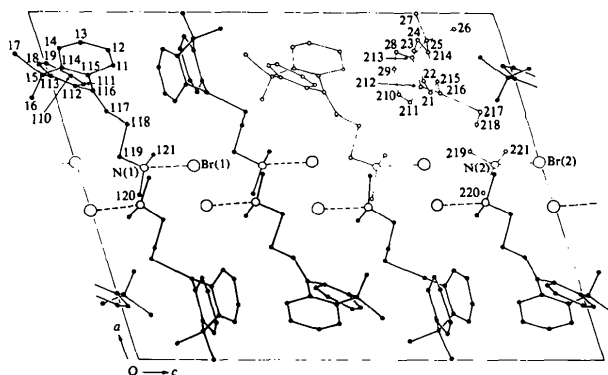

Fig. 1. The crystal structure of melitracene hydrobromide as seen along b.
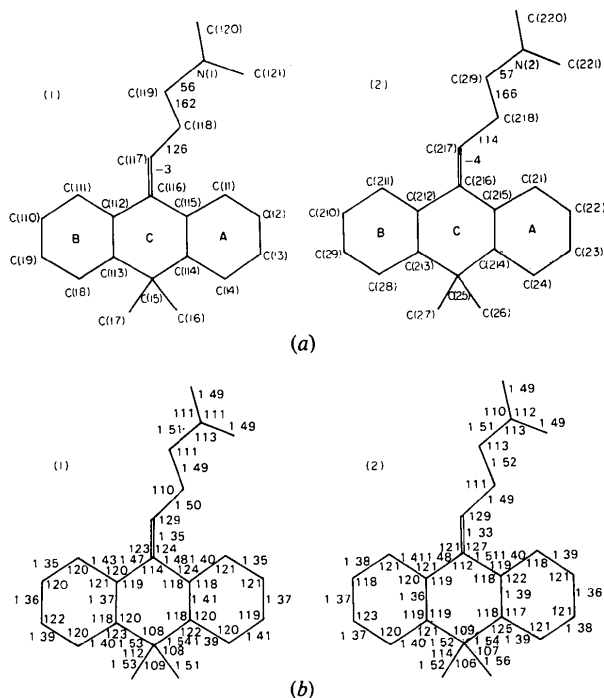
(a)

(b)

Fig. 2. The melitracene molecules 1 and 2. (a) Torsion angles, average e.s.d. 1°. (b) Bond distances and angles, average e.s.d.'s 0·015 Å and 1°. The tricyclic ring system of molecule 1 (2) is seen from its concave (convex) side.

conformation: C(112), C(113), C(114) and C(115) lie in a plane, C(15) and C(116) being 0·50 and 0·42 Å out of it, respectively. The same geometry is present in molecule 2.

The methyl groups are in the following positions: C(16), C(26) flagpole and C(17), C(27) bowsprit.

The distances C(116)—C(117) and C(216)—C(217) indicate absence of conjugation with the aromatic rings. Moreover, these bonds are out of the planes defined by the phenyl rings (Table 3).

From the pharmacological point of view and according to theories of structure–activity relationships (Horn, 1976; Rodgers, Horn & Kennard, 1975), the distances from N(1) and N(2) to the centers of the two phenyl rings are important. These values are 7·48 and 6·18 Å in molecule 1, and 7·46 and 6·08 Å in molecule 2. The angle between the two phenyl rings also seems to be important (Maxwell, Keenan, Chaplin,

Table 2. *The geometry of the hydrogen bonds* A—$H\cdots B$

E.s.d.'s are given in parentheses.

A–H$\cdots B$	A–H	H$\cdots B$	$A\cdots B$	AHB
N(1) H|N(1)|$\cdots$Br(1)	0·84 (18) Å	2·42 (17) Å	3·231 (8) Å	163 (15)°
N(2) H|N(2)|$\cdots$Br(2)	0·88 (15)	2·31 (15)	3·183 (7)	173 (15)

Table 3. *Deviations* (Å) *of the atoms involved in the double bonds from the planes defined by the phenyl rings*

Standard deviations are given in parentheses.

	Molecule 1			Molecule 2	
	Ring A	Ring B		Ring A	Ring B
C(116)	0·02 (1)	0·13 (1)	C(216)	0·003 (9)	0·030 (9)
C(117)	−0·69 (1)	−0·50 (1)	C(217)	0·666 (9)	0·744 (9)

Roth & Eckhardt, 1969), the corresponding values being here 137 (molecule 1) and 141° (molecule 2).

Most of the calculations were carried out with the XRAY 70 system (Stewart, Kundell & Baldwin, 1970). Thanks are due to the staff of the Centro de Proceso de Datos del Ministerio de Educación y Ciencia, Madrid, for the facilities provided on the 1108 Univac computer.

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