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Crystal and Molecular Structure of *N*-Tosyl-2,12-ethano-2-ethyl-8-methoxy-1,4-methylene-1,2,3,4,5,6,12,13-octahydrophenanthridin-3-one

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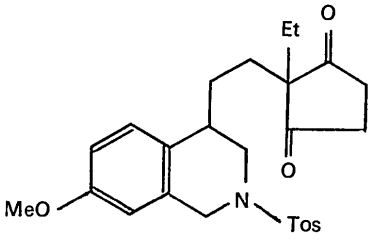
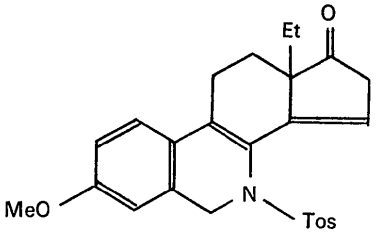
The structure of the title compound has been determined by single-crystal X-ray analysis from diffractometer data, and has been refined by least-squares calculations to an R of 0·066. The molecular geometry shows considerable evidence of steric strain, indicated both by large distortions of valency angles from ideal values, and also by C sp^3–C sp^3 bonds which are slightly, but significantly, longer than might otherwise be expected.

Introduction

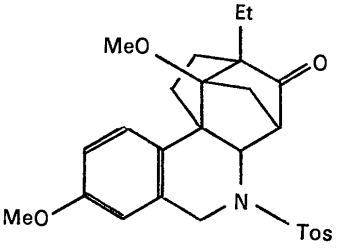
In the course of an attempted total synthesis of a 7-azasteroid, acid-catalysed (methanol saturated with hydrogen chloride gas) treatment of the diketone intermediate (I) yielded a product which was shown by n.m.r. and mass-spectrometric examination to differ from (II), the product to be expected on the basis of well established precedents (Anachenko & Torgov, 1959; Douglas *et al.*, 1963; Huisman, 1968, 1971). Moreover, the structure of the product could not be assigned unambiguously by chemical and spectroscopic techniques. Since it seemed likely that considerable skeletal rearrangement had taken place, we undertook an X-ray analysis which has proved that the molecular structure of the unknown product is (III).



(I)



(II)



(III)

In the present paper we record details of the analysis and discuss the salient features of the molecular geometry. Details of the synthesis of (I), and also of the principles underlying the rearrangement process which gives rise to (III), will be discussed elsewhere.

Experimental

Crystal data

$C_{27}H_{29}O_5NS$, $M=479·6$, monoclinic. $a=10·600(6)$, $b=21·840(13)$, $c=11·510(7)$ Å, $\beta=114·90(3)°$; $U=2416·8$ Å^3; $D_m=1·32$ g cm^{-3} (by flotation in aqueous KI), $Z=4$, $D_c=1·32$ g cm^{-3}, F (000) $=1016$. Space group $P2_1/c$. $\mu=1·75$ cm^{-1} (for Mo $K\alpha$, $\lambda=0·7107$ Å).

Crystallographic measurements

The cell parameters were determined initially from oscillation and Weissenberg photographs taken with Cu $K\alpha$ ($\lambda=1·5418$ Å) radiation, and from precession photographs taken with Mo $K\alpha$ radiation, and were later refined by least-squares techniques prior to the diffractometer data collection. Systematic absences in the $0k0$ and $h0l$ X-ray spectra uniquely determine the space group as $P2_1/c$.

Intensity measurements were made on a Hilger and Watts Y290 diffractometer, with a small needle-shaped crystal (0·2 × 0·5 × 0·2 mm) mounted about **b** and Zr-filtered Mo radiation. The θ–ω-scan technique was

used in the 2θ range $0 \rightarrow 54°$ to measure the intensities of 3103 ($I > 2\sigma_I$, $\sigma_I = \sqrt{I + B_1} + B_2$) independent reflexions. The intensities were corrected for Lorentz and polarization effects, but absorption effects were considered small and were ignored.

Structure determination

The structure was solved by application of direct methods with programs developed by Stewart (1967), and incorporated into the X-RAY 70 suite of programs. An initial E map based on 251 reflexions ($|E| > 1{\cdot}70$) revealed most of the structure, and the complete structure was obtained after two rounds of structure-factor and electron-density calculations. In these latter calculations an overall isotropic thermal parameter $U_{iso} = 0{\cdot}05$ Å^2 was assumed, and after each calculation the data were placed on an approximate absolute scale by equating $k\sum|F_o|$ and $\sum|F_c|$.

Structure refinement

The positional, vibrational and overall scale parameters were refined initially by full-matrix least-squares calculations and subsequently with the block-diagonal approximation (on introduction of anisotropic thermal parameters). The calculations converged after 9 cycles when R was 0·066 and R' ($= \sum w\Delta^2 / \sum w|F_o|^2$) was 0·0078.* Before the refinement of anisotropic thermal parameters, positions were calculated for all non-methyl hydrogen atoms, and contributions from these were included, but not refined, in all subsequent structure-factor calculations. Throughout the refinement it was not found necessary to apply other than unit weights to the data.

On convergence of the refinement, the calculation of an electron-density distribution and a difference synthesis revealed no errors in the structure, and the refinement was considered complete.

Fractional coordinates and thermal parameters are given in Table 1, while Table 2 contains all bond lengths, valency angles and pertinent intra- and intermolecular non-bonded distances. The estimated standard deviations in Tables 1 and 2 are derived from the inverse of the least-squares normal-equation matrix, and are best regarded as minimum values. Details of least-squares planes calculated for various portions of the molecular framework are given in Table 3. The atomic numbering scheme used in the analysis is shown in Fig. 1; Fig. 2 shows a projected view of the molecular packing.

Molecular geometry

The aromatic ring A of the molecule does not deviate markedly from planarity, and although C(7) and the methoxy group are both almost coplanar with the ring, C(9) deviates by $-0{\cdot}19$ Å. It may also be significant that while most of the internal valency angles of ring A

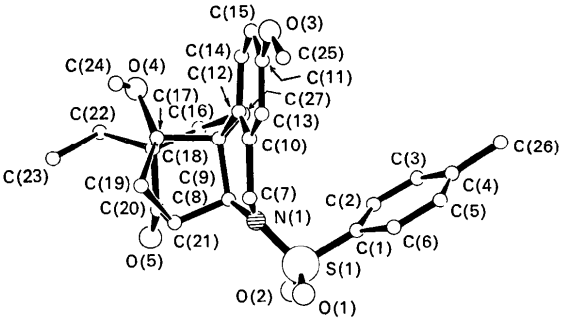


Fig. 1. A view of one molecule showing the atomic numbering.

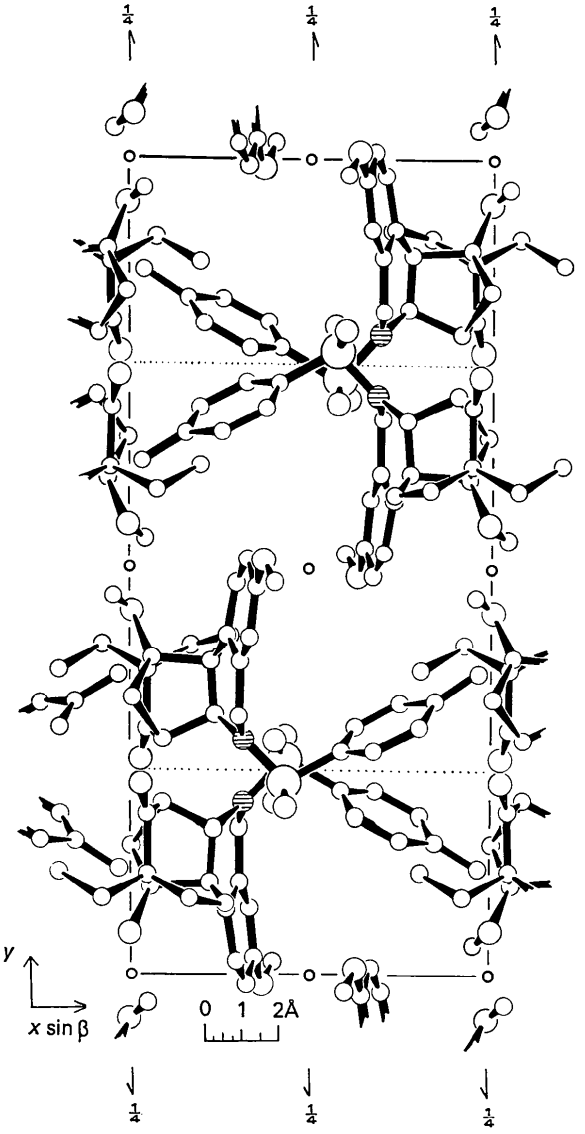


Fig. 2. The molecular packing viewed down **c**.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30437 (25 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

are acceptably close to 120°, the largest deviation is for angle C(10) C(12) C(14) [117·1(4)°], C(12) being the ring atom to which C(9) is bonded.

The conformation of the nitrogen-containing ring *B* is characterized by the approximately planar set of atoms C(7), C(8), C(9), C(10) and C(12), with the nitrogen atom 0·43 Å removed from this plane. Within ring *B*, the valency angles at C(9) [C(8) C(9) C(12) 115·5(3)°], C(8) [C(9) C(8) N(1) 114·6(3)°] and C(7) [C(10) C(7) N(1) 112·4(3)°] all show significant increases from ideal tetrahedral values, although the angles at C(10) and C(12) [C(7) C(10) C(12) 121·8(4)°, C(9) C(12) C(10) 121·9(4)°] differ little from 120°. It is probable that the conformation of ring *B* is largely dominated by the combined influence of the adjacent aromatic and fused-ring systems. The geometry of the nitrogen atom itself is that of a slightly flattened pyramid, with the sulphur atom displaced 0·25 Å from the plane defined by the nitrogen atom and atoms C(7) and C(8).

The three five-membered rings all adopt envelope conformations, with C(19) 0·84 Å distant from the plane of atoms C(8), C(9), C(17) and C(21), and 0·87 Å distant from the plane of atoms C(17), C(18), C(20), C(21) and O(5). The conformation of the third ring is consider-

Table 1. *Atomic parameters*

(*a*) Fractional coordinates

	x/a	*y/b*	*z/c*
S(1)	0·43044 (11)	0·23696 (5)	0·39911 (10)
O(1)	0·43295 (33)	0·20143 (14)	0·50482 (29)
O(2)	0·40147 (36)	0·20754 (14)	0·27972 (28)
O(3)	0·38025 (40)	0·51394 (16)	0·71146 (32)
O(4)	0·01108 (30)	0·45289 (12)	0·16920 (26)
O(5)	0·03020 (36)	0·27544 (15)	−0·05716 (29)
N(1)	0·31647 (35)	0·29069 (15)	0·37122 (30)
C(1)	0·59242 (34)	0·27389 (18)	0·44932 (37)
C(2)	0·62720 (49)	0·30325 (22)	0·35992 (41)
C(3)	0·75206 (54)	0·33406 (24)	0·40005 (48)
C(4)	0·84336 (49)	0·33632 (20)	0·52844 (47)
C(5)	0·80905 (49)	0·30594 (22)	0·616[illegible]2 (43)
C(6)	0·68324 (47)	0·27473 (21)	0·57812 (40)
C(7)	0·30120 (48)	0·31856 (19)	0·48037 (38)
C(8)	0·24739 (43)	0·31734 (18)	0·24185 (36)
C(9)	0·22842 (41)	0·38930 (18)	0·23913 (36)
C(10)	0·30975 (42)	0·38750 (19)	0·47963 (37)
C(11)	0·35085 (47)	0·48005 (21)	0·60209 (41)
C(12)	0·28294 (41)	0·42002 (19)	0·36822 (37)
C(13)	0·34404 (45)	0·41701 (20)	0·59648 (40)
C(14)	0·29623 (46)	0·48417 (20)	0·37875 (40)
C(15)	0·32929 (50)	0·51383 (21)	0·49324 (45)
C(16)	0·17207 (48)	0·40541 (23)	0·00911 (41)
C(17)	0·06510 (39)	0·39436 (17)	0·16393 (36)
C(18)	0·04342 (42)	0·37981 (18)	0·02500 (36)
C(19)	0·01065 (44)	0·33786 (19)	0·20741 (40)
C(20)	0·05291 (43)	0·30952 (19)	0·03150 (40)
C(21)	0·09689 (44)	0·29227 (18)	0·17043 (39)
C(22)	−0·09202 (47)	0·40299 (21)	−0·08394 (40)
C(23)	−0·22880 (53)	0·37731 (29)	−0·08733 (54)
C(24)	−0·04230 (55)	0·46157 (23)	0·26392 (50)
C(25)	0·40584 (69)	0·48091 (31)	0·82566 (49)
C(26)	0·97946 (58)	0·37184 (26)	0·57210 (60)
C(27)	0·28386 (45)	0·41739 (21)	0·14535 (40)

Table 1 (*cont.*)

(*b*) Anisotropic temperature factors (Å$^2 \times 10^4$)

	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{31}$	$2U_{12}$
S(1)	560	337	385	19	252	123
O(1)	663	441	579	291	370	42
O(2)	810	515	460	−286	224	251
O(3)	927	659	538	−364	400	15
O(4)	561	386	482	106	468	162
O(5)	800	527	478	−187	220	217
N(1)	523	427	369	137	298	250
C(1)	521	408	402	3	355	204
C(2)	602	653	449	164	461	256
C(3)	688	668	636	254	730	210
C(4)	576	453	702	−121	660	104
C(5)	581	601	513	−63	398	48
C(6)	621	558	422	87	406	18
C(7)	676	433	400	73	496	84
C(8)	488	384	381	75	286	65
C(9)	463	406	386	125	353	−4
C(10)	476	447	406	20	381	37
C(11)	562	559	456	−200	292	−18
C(12)	441	432	404	48	297	−7
C(13)	534	514	433	21	351	80
C(14)	575	440	462	54	287	−29
C(15)	628	460	597	−105	355	−41
C(16)	561	698	421	92	404	−84
C(17)	404	346	423	82	297	29
C(18)	480	421	360	66	258	8
C(19)	503	421	526	133	463	−3
C(20)	452	439	473	−12	224	96
C(21)	534	372	458	56	287	−8
C(22)	575	492	445	100	147	122
C(23)	492	921	767	279	220	64
C(24)	783	584	712	39	912	251
C(25)	1026	1039	435	−205	443	343
C(26)	696	648	1028	−207	816	−242
C(27)	496	534	477	155	416	−103

Mean estimated standard deviations (Å$^2 \times 10^4$)

	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{31}$	$2U_{12}$
S	6	5	5	8	9	9
O	22	18	18	29	32	32
N	20	19	17	29	30	31
C	27	26	25	38	40	40

Table 2. *Interatomic distances and angles with estimated standard deviations in parentheses*

(*a*) Bonded distances (Å)

S(1)—O(1)	1·434 (3)	C(8)—C(9)	1·583 (6)
S(1)—O(2)	1·428 (3)	C(8)—C(21)	1·554 (6)
S(1)—N(1)	1·616 (4)	C(9)—C(12)	1·506 (6)
S(1)—C(1)	1·760 (4)	C(9)—C(17)	1·580 (5)
O(3)—C(11)	1·378 (6)	C(9)—C(27)	1·556 (6)
O(3)—C(25)	1·422 (7)	C(10)–C(12)	1·387 (6)
O(4)—C(17)	1·412 (5)	C(10)–C(13)	1·395 (6)
O(4)—C(24)	1·437 (6)	C(11)–C(13)	1·379 (6)
O(5)—C(20)	1·203 (5)	C(11)–C(15)	1·387 (7)
N(1)—C(7)	1·465 (5)	C(12)–C(14)	1·408 (6)
N(1)—C(8)	1·474 (5)	C(14)–C(15)	1·375 (7)
C(1)—C(2)	1·388 (6)	C(16)–C(18)	1·554 (6)
C(1)—C(6)	1·387 (6)	C(16)–C(27)	1·538 (6)
C(2)—C(3)	1·380 (7)	C(17)–C(18)	1·550 (6)
C(3)—C(4)	1·385 (7)	C(17)–C(19)	1·533 (6)
C(4)—C(5)	1·386 (7)	C(18)–C(20)	1·538 (6)
C(4)—C(26)	1·525 (7)	C(18)–C(22)	1·541 (6)
C(5)—C(6)	1·393 (7)	C(19)–C(21)	1·528 (6)
C(7)—C(10)	1·509 (6)	C(20)–C(21)	1·513 (6)
C(22)–C(23)	1·540 (7)		

Table 2 (*cont.*)

(*b*) Interbond angles (°)

O(1)S(1)O(2)	119·5 (2)	O(1)S(1)N(1)	107·8 (2)
O(1)S(1)C(1)	107·6 (2)	O(2)S(1)N(1)	107·2 (2)
O(2)S(1)C(1)	107·8 (2)	N(1)S(1)C(1)	106·1 (2)
S(1)N(1)C(7)	118·3 (3)	S(1)N(1)C(8)	119·9 (3)
S(1)C(1)C(2)	119·7 (3)	S(1)C(1)C(6)	120·0 (3)
C(11)O(3)C(25)	117·0 (4)	O(3)C(11)C(13)	124·5 (4)
O(3)C(11)C(15)	115·3 (4)	C(17)O(4)C(24)	116·6 (3)
O(4)C(17)C(9)	114·2 (3)	O(4)C(17)C(18)	110·1 (3)
O(4)C(17)C(19)	120·0 (3)	O(5)C(20)C(18)	126·2 (4)
O(5)C(20)C(21)	127·3 (4)	C(7)N(1)C(8)	121·1 (3)
N(1)C(7)C(10)	112·4 (3)	N(1)C(8)C(9)	114·6 (3)
N(1)C(8)C(21)	111·0 (3)	C(2)C(1)C(6)	120·3 (4)
C(1)C(2)C(3)	119·6 (4)	C(1)C(6)C(5)	119·3 (4)
C(2)C(3)C(4)	121·0 (4)	C(3)C(4)C(5)	119·0 (4)
C(3)C(4)C(26)	120·6 (5)	C(5)C(4)C(26)	120·4 (4)
C(4)C(5)C(6)	120·7 (4)	C(7)C(10)C(12)	121·8 (4)
C(7)C(10)C(13)	116·6 (4)	C(9)C(8)C(21)	104·2 (3)
C(8)C(9)C(12)	115·5 (3)	C(8)C(9)C(17)	100·4 (3)
C(8)C(9)C(27)	108·9 (3)	C(8)C(21)C(19)	103·0 (3)
C(8)C(21)C(20)	105·2 (3)	C(12)C(9)C(17)	112·7 (3)
C(12)C(9)C(27)	114·1 (3)	C(9)C(12)C(10)	121·9 (4)
C(9)C(12)C(14)	120·7 (4)	C(17)C(9)C(27)	103·8 (3)
C(9)C(17)C(18)	101·7 (3)	C(9)C(17)C(19)	104·0 (3)
C(9)C(27)C(16)	106·6 (3)	C(12)C(10)C(13)	121·6 (4)
C(10)C(12)C(14)	117·1 (4)	C(10)C(13)C(11)	119·6 (4)
C(13)C(11)C(15)	120·2 (4)	C(11)C(15)C(14)	119·6 (4)
C(12)C(14)C(15)	121·8 (4)	C(18)C(16)C(27)	106·2 (3)
C(16)C(18)C(17)	106·9 (3)	C(16)C(18)C(20)	108·8 (3)
C(16)C(18)C(22)	110·4 (3)	C(18)C(17)C(19)	105·0 (3)
C(17)C(18)C(20)	100·2 (3)	C(17)C(18)C(22)	117·1 (3)
C(17)C(19)C(21)	94·7 (3)	C(20)C(18)C(22)	112·8 (3)
C(18)C(20)C(21)	106·5 (3)	C(18)C(22)C(23)	116·5 (4)
C(19)C(21)C(20)	100·3 (3)		

(*c*) Selected intramolecular non-bonded distances (Å) < 3·40 Å

O(1)····C(6)	2·90	C(8)····C(16)	3·12
O(1)····C(7)	2·87	C(8)····C(18)	2·87
O(2)····C(2)	3·01	C(9)····C(16)	2·48
O(2)····C(8)	2·83	C(9)····C(20)	2·91
O(4)····C(12)	2·92	C(9)····C(24)	3·39
O(4)····C(14)	3·05	C(14)···C(17)	3·30
O(4)····C(22)	2·86	C(14)···C(24)	3·30
O(5)····C(16)	3·15	C(14)···C(27)	3·01
O(5)····C(22)	3·03	C(16)···C(21)	3·38
N(1)····C(2)	3·36	C(17)···C(23)	3·26
N(1)····C(12)	2·85	C(19)···C(22)	3·37
N(1)····C(19)	3·16	C(19)···C(23)	3·38
C(7)····C(9)	2·98	C(19)···C(24)	2·89
C(7)····C(19)	3·37	C(20)···C(23)	3·09
C(8)····C(10)	2·96	C(20)···C(27)	3·25

Table 2 (*cont.*)

(*d*) Intermolecular distances (Å) < 3·85 Å

C(2)····O(1^{i})	3·72	C(16)···O(4^{vi})	3·77
C(3)····O(3^{ii})	3·62	C(19)···O(5^{v})	3·61
C(3)····O(5^{iii})	3·67	C(19)···C(5^{vii})	3·69
C(4)····O(5^{iii})	3·54	C(21)···C(4^{vii})	3·75
C(5)····O(5^{iv})	3·55	C(21)···C(5^{vii})	3·57
C(7)····O(5^{v})	3·41	C(21)···O(5^{vii})	3·79
C(7)····O(2^{v})	3·20	C(22)···O(4^{vi})	3·51
C(10)···O(2^{v})	3·78	C(22)···C(5^{viii})	3·79
C(13)···O(2^{v})	3·34	C(24)···O(3^{ix})	3·75
C(14)···C(11^{ii})	3·74	C(25)···C(24^{ix})	3·76
C(15)···C(3^{ii})	3·77	C(26)···O(5^{iii})	3·67
C(15)···C(4^{ii})	3·71	C(26)···C(21^{iii})	3·81
C(15)···C(14^{ii})	3·61	C(27)···O(1^{i})	3·74
C(15)···C(15^{ii})	3·61	C(27)···O(3^{ii})	3·56
C(16)···O(1^{i})	3·63	N(1)····O(5^{iii})	3·75

Superscript roman numerals refer to the following equivalent positions, which should be applied to the coordinates of the second atom:

i	x,	$\frac{1}{2}+y$,	$-\frac{1}{2}+z$
ii	$1-x$,	$1-y$,	$1-z$
iii	$1+x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$
iv	$1+x$,	y,	$1+z$
v	x,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$
vi	$-x$,	$1-y$,	$-z$
vii	$-1+x$,	$\frac{1}{2}-y$,	$-\frac{1}{2}+z$
viii	$-1+x$,	y,	$-1+z$
ix	$-x$,	$1-y$,	$1-z$

Table 3. *Least-squares planes given in the form* $lX'+mY'+nZ'=d'$, *where* X', Y' *and* Z' *are coordinates in* Å

(*a*) Plane equations

Plane (1): $+0{\cdot}541X' - 0{\cdot}833Y' - 0{\cdot}118Z' = -3{\cdot}312$
Plane (2): $+0{\cdot}979X' - 0{\cdot}060Y' + 0{\cdot}198Z' = +1{\cdot}413$
Plane (3): $-0{\cdot}985X' + 0{\cdot}007Y' - 0{\cdot}175Z' = -1{\cdot}734$
Plane (4): $-0{\cdot}406X' + 0{\cdot}912Y' + 0{\cdot}054Z' = +7{\cdot}411$
Plane (5): $+0{\cdot}499X' + 0{\cdot}043Y' - 0{\cdot}865Z' = -1{\cdot}166$
Plane (6): $-0{\cdot}978X' - 0{\cdot}092Y' - 0{\cdot}185Z' = -1{\cdot}075$
Plane (7): $+0{\cdot}802X' + 0{\cdot}569Y' + 0{\cdot}183Z' = +5{\cdot}565$

Table 3 (*cont.*)

(*b*) Deviations of atoms (Å) from planes (starred atoms not used to define planes)

Plane (1):	C(1)	−0·007	C(2)	0·004	C(3)	0·004
	C(4)	−0·009	C(5)	0·006	C(6)	0·002
	C(26)*	−0·043	S(1)*	−0·070		
Plane (2):	C(10)	0·006	C(11)	−0·017	C(12)	−0·016
	C(13)	0·010	C(14)	0·010	C(15)	0·007
	O(3)*	−0·050	C(25)*	−0·047	C(7)*	0·006
	C(9)*	−0·195				
Plane (3):	C(7)	0·058	C(8)	−0·085	C(9)	0·117
	C(10)	−0·023	C(12)	−0·067	N(1)*	−0·428
Plane (4):	C(9)	−0·032	C(16)	−0·051	C(18)	0·033
	C(27)	0·051	C(17)*	0·581		
Plane (5):	C(8)	0·001	C(9)	−0·001	C(17)	0·001
	C(21)	−0·001	C(19)*	−0·838		
Plane (6):	C(17)	0·067	C(18)	−0·069	C(20)	−0·008
	C(21)	−0·039	O(5)	0·048	C(19)*	0·868
Plane (7):	C(7)	0·000	C(8)	0·000	N(1)	0·000
	S(1)*	0·246				

ably more flattened, with C(17) only 0·58 Å removed from the plane of C(9), C(12), C(16) and C(18). There is considerable evidence of molecular strain in this region of the molecule. In particular, two of the bonds radiating from C(9) [C(9)–C(8) 1·583(6) Å; C(9)–C(17) 1·580(5) Å] are significantly longer than might otherwise be expected for similar bond types in a less restricted environment. For the C(9)–C(8) bond the substituents on both atoms are fully eclipsed, while for the C(9)–C(17) bond, although there is slight staggering, both atoms are fully substituted by relatively bulky groups. Similar lengthening of C sp^3–C sp^3 bonds has been noted in similar molecules where comparable constraints exist (Cameron, Hair, Greengrass & Ramage, 1974; Beisler, Silverton, Penttila, Horn & Fales, 1971; Gilardi, 1972). In the same context, the valency angles about C(9) [100·4→115·5°], C(8) [104·2→114·6°], C(17) [101·7→120·0°] and C(18) [100·2→117·1°] show considerable distortions from tetrahedral values, the smaller angles in general being endocyclic with respect to the fused ring system, while the larger angles are exocyclic. The relative values of the angles are also in accord with those which would be expected to arise both from the restrictions of the cyclic system, and also from the interactions of bulky substituents.

Other dimensions within the molecule compare well with literature values for similar bonding situations. There are no abnormally short intermolecular distances, and the molecular packing would therefore appear to be dominated largely by van der Waals forces.

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X-ray Diffraction from Fatty-Acid Multilayers. Significance of Intensity Data in Low-Angle Diffraction

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X-ray diffraction has been recorded from various fatty-acid multilayer systems (barium stearate, barium myristate, magnesium stearate at 0 and 100% relative humidity). The multilayers are treated as simple trial structures for low-angle diffraction experiments with biological membranes. Spacings and intensities of reflexions are analysed. Fourier syntheses calculated with scaled amplitudes of the structure factors provide electron-density functions of the bilayer profiles which are on an absolute scale of electron density.

Introduction

Planar multilamellar systems (multilayers) can be prepared with salts of long-chain fatty acids by the technique of Blodgett (1935). These multilayers are built up by dipping a solid support such as a flat glass plate through a monomolecular film of the fatty acid spread on the surface of an electrolyte solution. Successive monomolecular layers are then transferred onto the support every time it passes through the monomolecular film. The molecules in the multilayer are overturned in every other layer so that a plane of symmetry exists between two neighbouring monolayers. Multilayers, then, consist of a sequence of stacked and parallel bilayers.

The electron density of a multilayer will be called $g(\mathbf{r})$. The normal to the plane of the bilayers is defined as the z axis and the structure will have rotational symmetry and constant radius around z. $g(\mathbf{r})$ in cylindrical coordinates is then

$$g(r,\varphi,z)=u(r)\,.\,\varrho(z)$$

where $u(r)$ is the density function in the bilayer plane. In the following discussion $u(r)$ is assumed to be con-