where, however, the P—N distances are much shorter [1·695 (4) Å], and the P···P (2·52) and N···N (2·25 Å) non-bonded interactions across the ring are said to distort its shape from a regular square. In the present compound the non-bonded distances are P(1)···P(1)' (2·53) and N(2)···N(2)' (2·48 Å). The longer N···N contact distance is consistent with the increased space required to accommodate an sp^3 rather than an sp^2 N atom (Coulson, 1961).

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6-*N*-Dimethylaminonaphthylsulphonylaziridine

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Abstract. $C_{14}H_{16}N_2O_2S$, monoclinic, space group $P2_1/a$, $Z = 4$, $a = 22·277$ (2), $b = 7·469$ (2), $c = 8·001$ (1) Å, $\beta = 100·18$ (8)°, final $R = 0·040$ for 1233 intensities with $I > \sigma(I)$. The naphthalene system is not planar; the sulphone-group tetrahedron is very distorted with evidence of interaction between S d_{xy} and C $p\pi$ orbitals. The aziridene group shows the angles, but not bond lengths, expected from other measurements of systems containing this group. The *N*-dimethylamino group has the usual geometry.

Introduction. The commercial product (Pierce, Rockford, Illinois) was crystallized by cooling an ethanol–water solution. Intensities were collected on a Philips PW 1100 four-circle diffractometer. 1379 independent reflexions were measured in the Cu sphere in the $\theta/2\theta$ scan mode.

The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). The positions and anisotropic thermal factors of all non-hydrogen atoms were refined by full-matrix least squares. During the refinement it was possible to locate the H atoms on a difference synthesis; in the last cycle they were refined isotropically. Table 1 lists the fractional atomic coordinates and ther-

mal parameters, Table 2 the bond angles and Table 3 the bond lengths.*

Discussion. The title compound (*N*-dansylaziridine) (Fig. 1) is an activated molecule belonging to the group of aziridines which easily react with nucleophiles. It is a fluorescent selective reagent towards thiolic groups and finds its main use in biochemistry as a marker of cysteines present in proteins (Scouten, Lubcher & Baughman, 1974).

Naphthalene system. The usual distribution of bond lengths is observed (Aleby, 1972; Cruickshank, 1957). The mean C_{sp^2}—C_{sp^2} length is 1·402 (3) and the mean C_{sp^2}—H distance 0·97 (9) Å.

The internal angle at the S-substituted C atom is 121·5 (3)° in good agreement with values reported for phenyl sulphones (Domenicano, Vaciago & Coulson, 1975). The naphthalene system is not planar: the

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31969 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Fractional atomic coordinates* $(\times 10^5, for$ H $\times$ $10^4)$ *and thermal parameters* $(\times 10^5$ *except for* H$)$
with standard deviations in parentheses

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	31523 (15)	87009 (45)	71628 (45)	135 (9)	865 (74)	1186 (74)	24 (20)	99 (21)	70 (59)
C(2)	29305 (18)	81123 (51)	55816 (51)	181 (11)	1367 (87)	1288 (83)	21 (24)	246 (26)	−179 (68)
C(3)	23134 (18)	80209 (52)	49785 (50)	220 (12)	1438 (92)	1004 (73)	−92 (25)	108 (26)	−151 (66)
C(4)	19078 (17)	84954 (50)	59446 (46)	151 (9)	1559 (85)	1256 (77)	−79 (24)	52 (23)	91 (64)
C(5)	21036 (15)	90256 (45)	76234 (41)	144 (9)	840 (71)	986 (71)	39 (20)	94 (20)	26 (58)
C(6)	17108 (14)	93692 (47)	87904 (42)	123 (8)	1084 (76)	1000 (72)	46 (21)	51 (20)	74 (60)
C(7)	19295 (17)	97825 (51)	104111 (53)	146 (11)	1311 (85)	1582 (92)	67 (23)	254 (27)	11 (67)
C(8)	25457 (17)	98539 (52)	110224 (49)	178 (11)	1452 (88)	1039 (75)	12 (23)	86 (24)	−87 (65)
C(9)	29353 (17)	95268 (47)	99503 (45)	1150 (9)	1153 (81)	1233 (79)	26 (22)	21 (23)	−67 (62)
C(10)	27345 (14)	91328 (45)	82453 (41)	108 (8)	892 (70)	1074 (68)	26 (20)	71 (19)	26 (59)
N(11)	37723 (12)	88249 (43)	78370 (38)	111 (7)	1799 (81)	1713 (63)	52 (20)	168 (18)	−157 (57)
C(12)	40017 (21)	106411 (70)	80987 (79)	147 (12)	2169 (121)	2893 (131)	−173 (31)	77 (32)	−57 (107)
C(13)	41714 (13)	77332 (90)	70055 (76)	188 (13)	3456 (16)	2318 (124)	251 (37)	299 (32)	−579 (122)
S(14)	9247 (4)	91502 (14)	82459 (13)	96 (2)	1505 (23)	1576 (20)	5 (6)	119 (5)	281 (19)
O(15)	7712 (11)	75753 (38)	72530 (37)	162 (7)	1764 (63)	2681 (68)	−131 (17)	115 (16)	−154 (58)
O(16)	67642 (11)	93450 (40)	97428 (33)	153 (6)	2693 (74)	1953 (56)	101 (18)	273 (15)	610 (55)
N(17)	7465 (13)	108805 (45)	69623 (38)	139 (8)	1916 (78)	1535 (62)	84 (20)	100 (16)	262 (62)
C(18)	1233 (18)	115306 (63)	68439 (65)	123 (10)	2087 (105)	183 (98)	98 (23)	40 (28)	106 (87)
C(19)	6182 (20)	125625 (66)	77491 (61)	232 (12)	1821 (108)	1621 (96)	30 (31)	41 (27)	94 (92)

	x	y	z	B (Å^2)		x	y	z	B (Å^2)
H(102)	3195 (15)	7765 (46)	4941 (42)	2·6 (8)	H(312)	4030 (22)	11195 (72)	7031 (66)	7·7 (16)
H(103)	2142 (15)	7429 (49)	3839 (45)	3·8 (8)	H(113)	4595 (22)	7637 (65)	7854 (57)	6·7 (12)
H(104)	1457 (16)	8420 (44)	5548 (39)	2·8 (7)	H(213)	4206 (18)	8198 (57)	5914 (55)	4·9 (11)
H(107)	1671 (16)	10013 (49)	11016 (44)	3·2 (9)	H(313)	3395 (23)	6456 (75)	6754 (64)	8·2 (16)
H(108)	2733 (15)	9171 (46)	12200 (45)	3·1 (8)	H(118)	−116 (15)	10980 (45)	7490 (40)	2·1 (8)
H(109)	3349 (15)	9558 (40)	10390 (37)	1·8 (7)	H(218)	−85 (18)	11764 (55)	5751 (50)	4·7 (11)
H(112)	4432 (21)	10592 (60)	8852 (52)	6·1 (11)	H(119)	762 (18)	13626 (62)	7225 (52)	5·3 (11)
H(212)	3703 (22)	11360 (66)	8710 (57)	7·1 (13)	H(219)	638 (17)	12726 (58)	9029 (56)	5·5 (11)

Table 2. *Bond angles* (°)

C(1)–C(2)–C(3)	121·5 (4)	C(8)–C(9)–C(10)	122·1 (3)	C(2)–C(1)–C(11)	123·9 (3)
C(2)–C(3)–C(4)	121·4 (4)	C(9)–C(10)–C(5)	119·0 (3)	C(5)–C(6)–S(14)	122·3 (3)
C(3)–C(4)–C(5)	120·2 (3)	C(10)–C(1)–C(2)	118·5 (3)	O(16)–S(14)–C(6)	107·9 (2)
C(4)–C(5)–C(10)	118·6 (3)	O(15)–S(14)–O(16)	117·9 (2)	O(15)–S(14)–C(6)	110·5 (2)
C(5)–C(6)–C(7)	121·5 (3)	C(18)–N(17)–C(19)	60·0 (3)	O(15)–S(14)–N(17)	106·0 (2)
C(5)–C(10)–C(1)	119·7 (3)	C(19)–C(18)–N(17)	59·9 (3)	O(16)–S(14)–N(17)	111·4 (2)
C(6)–C(5)–C(10)	117·0 (3)	C(18)–C(19)–N(17)	60·1 (3)	S(14)–N(17)–C(19)	115·9 (3)
C(6)–S(14)–N(17)	101·9 (2)	C(1)–N(11)–C(13)	115·8 (3)	S(14)–N(17)–C(18)	114·6 (3)
C(6)–C(7)–C(8)	121·3 (4)	C(1)–N(11)–C(12)	115·0 (3)		
C(7)–C(8)–C(9)	119·0 (4)	C(13)–N(11)–C(12)	110·4 (4)		

calculated least-squares planes through the atoms of rings A and B respectively have equations:

$$0\cdot8188X + 7\cdot2690Y - 1\cdot8740Z - 5\cdot3081 = 0$$

$$1\cdot3448X + 7\cdot0832Y - 2\cdot5841Z - 4\cdot7151 = 0.$$

The angle between these two planes is 5·2°; the displacements of C(7), C(8), C(2), C(3) from the best plane calculated with the ten C atoms of the aromatic ring indicate that the system is slightly folded in a butterfly-wing conformation. The origin of this deviation from planarity could lie in intramolecular van der Waals (*peri*) interactions. The distance between the H atom bonded to C(4) and O(15) is 2·34 (3) Å, whilst the sum of the van der Waals radii is 2·60 Å.

Similar conclusions can be drawn from the distance

Table 3. *Bond distances* (Å)

C(1)–C(10)	1·440 (5)	C(6)–S(14)	1·764 (3)
C(1)–C(2)	1·368 (5)	S(14)–O(15)	1·434 (3)
C(2)–C(3)	1·398 (6)	S(14)–O(16)	1·437 (3)
C(3)–C(4)	1·359 (5)	S(14)–N(17)	1·665 (3)
C(4)–C(5)	1·415 (5)	N(17)–C(18)	1·479 (3)
C(5)–C(6)	1·436 (5)	N(17)–C(18)	1·463 (6)
C(6)–C(7)	1·359 (5)	C(18)–C(19)	1·448 (6)
C(7)–C(8)	1·396 (6)	N(11)–C(1)	1·416 (4)
C(8)–C(9)	1·369 (5)	N(11)–C(12)	1·454 (6)
C(9)–C(10)	1·411 (5)	N(11)–C(13)	1·469 (7)
C(10)–C(5)	1·430 (5)		

between the same H atom and S: in this case the value of 2·74 (3) found is 0·28 Å less than the theoretical one.
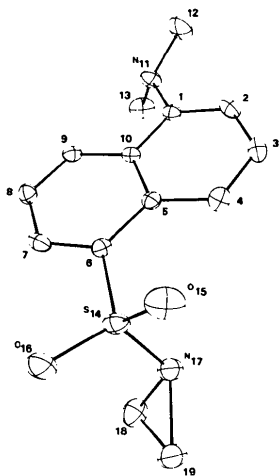
Fig. 1. *ORTEP* plot (Johnson, 1965) of *N*-dansylaziridine: ring *A* contains C(6), ring *B* C(4). Ellipsoids are scaled to include 25% probability.

Finally, another interaction can be observed between one of the H atoms of C(13) and the H atom bonded to C(9); the value for the distance H(113)—H(109) of 2·17 (6) is 0·23 Å less than the sum of the van der Waals radii. There are no other short intermolecular contacts.

Sulphone group. A C—S length of 1·764 (3) Å is observed while in non-aromatic compounds values of 1·82 Å are found. (McGregor & Speakman, 1969). This value and others reported (Sime & Abrahams, 1960) underline that in this case there must be interaction between d_{xy} orbitals of S and $p\pi$ orbitals of C (Koch & Moffitt, 1951).

The same conclusion is suggested by the angle between ring *A* and the C(6)—S(14)—N(17) plane, 68·1°, a value at which some delocalization should still be possible.

The tetrahedron of the sulphone group is very distorted, as often happens in phenyl sulphones (Sime & Abrahams, 1960); the S—O lengths show clear double-bond character.

The N—S distance is equal to that found in other sulphonyl aziridines (Trefonas & Majeste, 1965; Tulinsky & van den Hende, 1967).

Aziridine group. The only reported example of such a system, not condensed to other cyclic formations, is that of ethyleneimine, C_2H_5N, studied by means of microwaves (Tuner, Fiora & Kendrick, 1955) and the recent report (Delugeard, Vaultier & Meinnel, 1975) in which C atoms are partially substituted. However,

several structure determinations of systems in which the aziridine is condensed with saturated rings can be found. From these it has been concluded that both C—C and C—N lengths tend to increase as the number of C atoms of the fused ring increases, reaching values as high as 1·52 Å for the C—C distance when the ring is cyclododecane (Trefonas, Towns & Majeste, 1967; Zacharis & Trefonas, 1968). In every case however, the angles tend to be close to 60°. In *N*-dansylaziridine the values of the angles follow this scheme but bond lengths deviate significantly from other measurements. Considering that C(19) and C(18) are not fused to a ring one would expect values close to those reported by Tuner *et al.* (1955): 1·488 for C—C and 1·480 Å for C—N. The values found in *N*-dansylaziridine are C(18)—C(19) 1·448 (6), C(19)—N(17) 1·463 (6) and C(18)—N(17) 1·479 (3) Å.

N-Dimethylamino group. This substituent showed no features different from the values commonly reported. Bond lengths are listed in Table 3 and the angle between ring *B* and the C(1)—C(13)—C(12) plane is 48·7°.

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