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# The Structure of Diethyl 1-(*p*-Methoxyphenylsulphonyl)-2,2-aziridinedicarboxylate, $C_{15}H_{19}NO_7S$

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**Abstract.** $M_r = 357\cdot4$, monoclinic, $P2_1/c$, $a = 17\cdot124\,(2)$, $b = 10\cdot364\,(1)$, $c = 10\cdot144\,(1)$ Å, $\beta = 106\cdot41\,(3)°$, $V = 1727\cdot0\,(4)$ Å$^3$, $Z = 4$, $D_x = 1\cdot374$ g cm$^{-3}$, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 2\cdot122$ cm$^{-1}$, $F(000) = 752$, room temperature, final $R = 0\cdot041$ for 1347 observed reflections. The N ring atom lies 0·700 (3) Å out of the plane of its three substituents and the N—S bond makes a mean valence angle of 117·6 (3)° with the two N—C bonds of the three-membered ring. The lone pair of this N atom is *trans* to O(5) across the S—N bond.

**Introduction.** The structure of the title compound was determined as part of a continuing study on aziridine systems in order to investigate the pyramidal structure of the ring N atom and the change of geometry in several different *N*-substituted compounds. The structures of non-substituted 2,2-aziridinedicarboxamide (Brückner, 1982), 1-methyl- and 1-phenyl-2,2-aziridinedicarboxamide (Brückner, Malpezzi, Prosyanik & Bondarenko, 1985) have been previously determined.

**Experimental.** Colourless crystal, 0·4 × 0·4 × 0·05 mm, Philips PW1100 diffractometer, graphite-monochromated Mo $K\alpha$, cell constants by least-squares analysis of $\theta$ angles of 21 strong reflections with $7 \leq \theta \leq 16°$; 3033 independent reflections $-17 \leq h \leq 17$, $0 \leq k \leq 10$, $0 \leq l \leq 12$ with $\theta \leq 25°$, 1347 with $I \geq 2\cdot5\sigma(I)$; $\theta/2\theta$ scan technique, three periodically monitored reflections with no intensity variation; Lp correction, absorption ignored; direct methods (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), 296 normalized structure factors with $|E| \geq 1\cdot69$; anisotropic blocked full-matrix refinement, isotropic for H [some located from difference electron density map and those of methyl groups involving C(6), C(8) and C(15) calculated], phenyl group treated as rigid body, 271 parameters refined; function minimized $\sum w(|F_o|^2 - |F_c|^2)$ with $w = 1\cdot5739\,[\sigma^2(F_o) + 0\cdot00007 \times (F_o)^2]^{-1}$; final $R = 0\cdot041$ and $R_w = 0\cdot033$; final $\Delta\rho$ excursion $-0\cdot22$–$0\cdot19$ e Å$^{-3}$, $(\Delta/\sigma)_{\text{mean}} = 0\cdot119$, $S = 1\cdot31$; refinement calculations with *SHELX*76 (Sheldrick, 1976); atomic scattering factors as supplied by the program.†

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† Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39772 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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**Discussion.** The atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1 and the atomic numbering scheme is given in Fig. 1. Table 2 lists bond distances, bond angles and selected torsion angles.

The three-membered heterocyclic ring is a regular triangle within experimental error, with a mean side of 1·484 (5) Å. This symmetry appears to be the result of a summation of asymmetries induced by different single effects such as the introduction of a heteroatom into a small ring (Allen, 1982, 1984) and the geometric variation due to each individual substituent (Allen, 1981; Lauher & Ibers, 1975; Jason & Ibers, 1977; Bak & Shaarup, 1971, 1972; Deakyne, Allen & Laurie, 1977). The N—C bond lengths are significantly longer than those found in 1-methyl and 1-phenyl compounds while the C(3)—C(4) bond exhibits no variation. The N atom is pyramidal lying 0·700 (3) Å out of the plane of its three substituents; the S—N bond of 1·675 (4) Å makes an angle of 122·4 (3)° with the aziridine plane and has a mean valence angle at N of 117·6 (3)°. This geometry is close to that found in other sulphonylaziridines (Bolognesi & Rossi, 1977; Tulinsky & van den Hende, 1967; Trefonas & Majeste, 1965). The S—N bond length is shorter than 1·73 Å, the expected value for a single bond (Jordan, Smith, Lohr & Lipscomb, 1963; Kimura, Watson, Davis, Lamendola & Nadir, 1979; Chen, Watson, Davis, Lamendola & Nadir, 1978) but is greater than the value found in some sulphonamides (Eliopoulos, Sheldrick & Hamodrakas, 1983; Hamodrakas, Akrigg, Sheldrick & Camoutsis, 1978). The S—O(5) and S—O(6) bond lengths of 1·434 (3) and 1·426 (3) Å show clear double-bond character.

The phenyl ring is almost parallel to the O(5)···O(6) direction as indicated by the contact distances C(10)···O(5) and C(14)···O(6) [2·942 (5) and 2·986 (5) Å, respectively] and by the torsion angles of Fig. 2. An analogous conformation was found in 2-(*p*-toluenesulphonyl)-3-(*p*-chlorophenyl)oxaziridine (Kimura *et al.*, 1979) and in 2-(*p*-toluenesulphonyl)-3-(*m*-nitrophenyl)oxaziridine (Chen *et al.*, 1978). The methoxy group is coplanar with the phenyl ring with a torsion angle around the O(7)—C(12) bond of 2·1 (6)°. The planar arrangement, observed in many structures, induces an enlargement of the C(11)—C(12)—O(7) angle [125·1 (4)°] and a narrowing of the C(13)—C(12)—O(7) angle [115·7 (4)°] with a tendency peculiar to this kind of system, as already shown by Di Rienzo, Domenicano, Portalone & Vaciago (1976) and Domiano, Nardelli, Balsamo, Macchia & Macchia (1979). This effect could be connected with some degree of conjugation between the O atom and the phenyl ring with the consequent shortening of the C(Ph)—O bond.

The plane defined by C(1)—C(4)—C(2) is nearly perpendicular to the ring plane, the twist being 87·1 (3)°, and the two planes nearly bisect the angles N—C(4)—C(3) and C(1)—C(4)—C(2). The bent-back angle between the normal to the C(1)—C(4)—C(2) plane and the C(3)—C(4) vector (Stalick & Ibers, 1970; Allen, 1981) is 60·3 (3)°. A similar conformation was found also in 1-methyl- and 1-phenylaziridines.

The two ethoxycarbonyl groups are planar with an angle between the two planes of 83·1 (2)°. These groups are differently oriented with respect to the aziridine ring as can be seen from the Newman projection of Fig. 2. The ethoxycarbonyl group that is *cis* to the sulphonyl group across the C(4)—N bond makes an angle of 54·1 (2)° with the aziridine ring, while the other group [which is 144·2 (3)° to the sulphonyl across C(4)—N] makes a corresponding angle of 77·1 (2)°. This difference was also found in dimethyl 2-(*p*-toluenesulphonyl)-1,1-cyclopropanedicarboxylate (Iwasaki, Mitamura & Tsuchihashi,

Table 1. *Fractional atomic coordinates* (×10⁴) *and equivalent isotropic thermal parameters* (Å²)

| | $x$ | $y$ | $z$ | $B_{eq}$† |
|---|---|---|---|---|
| S | 1601 (1) | 1035 (1) | 4403 (1) | 3·6 (1) |
| O(1) | 2773 (2) | −1273 (3) | 7292 (3) | 5·8 (3) |
| O(2) | 3241 (2) | 661 (3) | 6858 (3) | 4·3 (3) |
| O(3) | 4211 (2) | −1339 (4) | 5623 (3) | 7·0 (4) |
| O(4) | 3611 (1) | −822 (3) | 3438 (3) | 4·5 (3) |
| O(5) | 1368 (2) | 566 (3) | 5567 (3) | 4·3 (2) |
| O(6) | 2002 (2) | 2252 (2) | 4503 (3) | 4·5 (3) |
| O(7) | −1245 (1) | 1145 (3) | −421 (2) | 4·3 (2) |
| N | 2211 (2) | −17 (3) | 3921 (3) | 3·2 (3) |
| C(1) | 2928 (3) | −513 (4) | 6527 (5) | 4·1 (4) |
| C(2) | 3633 (3) | −1000 (4) | 4719 (5) | 4·2 (4) |
| C(3) | 2082 (3) | −1403 (4) | 4163 (4) | 4·0 (4) |
| C(4) | 2823 (2) | −737 (4) | 5001 (4) | 3·4 (3) |
| C(5) | 3338 (4) | 1082 (6) | 8267 (5) | 5·3 (5) |
| C(6) | 3645 (3) | 2434 (5) | 8403 (5) | 6·6 (5) |
| C(7) | 4351 (3) | −1145 (7) | 3051 (6) | 5·9 (6) |
| C(8) | 4291 (3) | −534 (6) | 1721 (6) | 7·8 (6) |
| C(9) | 760 (2) | 1017 (4) | 2975 (4) | 3·1 (6) |
| C(10) | 77 (3) | 289 (4) | 2961 (5) | 4·2 (4) |
| C(11) | −601 (3) | 314 (4) | 1850 (5) | 4·1 (4) |
| C(12) | −612 (2) | 1052 (4) | 722 (4) | 3·5 (3) |
| C(13) | 72 (3) | 1786 (4) | 725 (5) | 3·9 (4) |
| C(14) | 749 (3) | 1765 (4) | 1831 (5) | 3·8 (4) |
| C(15) | −1971 (2) | 462 (4) | −453 (4) | 4·9 (4) |

† $B_{eq} = \frac{1}{3}\sum_i\sum_j B_{ij}a^*_i a^*_j \mathbf{a}_i.\mathbf{a}_j$.

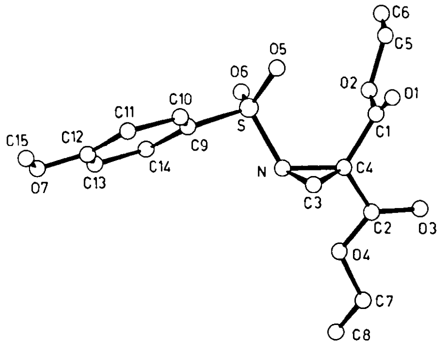

Fig. 1. Perspective view of the molecule showing atomic labelling.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°)

| | | | |
|---|---|---|---|
| S–O(5) | 1·434 (3) | N–C(4) | 1·485 (5) |
| S–O(6) | 1·426 (3) | C(1)–C(4) | 1·525 (6) |
| S–N | 1·675 (4) | C(2)–C(4) | 1·519 (7) |
| S–C(9) | 1·730 (3) | C(3)–C(4) | 1·483 (5) |
| O(1)–C(1) | 1·187 (6) | C(5)–C(6) | 1·490 (8) |
| O(2)–C(1) | 1·334 (5) | C(7)–C(8) | 1·468 (9) |
| O(2)–C(5) | 1·459 (6) | C(9)–C(10) | 1·390 (6) |
| O(3)–C(2) | 1·196 (5) | C(9)–C(14) | 1·391 (6) |
| O(4)–C(2) | 1·302 (6) | C(10)–C(11) | 1·371 (6) |
| O(4)–C(7) | 1·468 (7) | C(11)–C(12) | 1·372 (6) |
| O(7)–C(12) | 1·349 (4) | C(12)–C(13) | 1·396 (6) |
| O(7)–C(15) | 1·423 (5) | C(13)–C(14) | 1·367 (6) |
| N–C(3) | 1·484 (5) | | |
| | | N–C(3)–C(4) | 60·1 (2) |
| N–S–C(9) | 100·9 (2) | C(2)–C(4)–C(3) | 119·2 (4) |
| O(6)–S–C(9) | 109·8 (2) | C(1)–C(4)–C(3) | 119·3 (4) |
| O(6)–S–N | 105·6 (2) | C(1)–C(4)–C(2) | 111·5 (4) |
| O(5)–S–C(9) | 109·1 (2) | N–C(4)–C(3) | 60·0 (2) |
| O(5)–S–N | 111·2 (2) | N–C(4)–C(2) | 116·2 (3) |
| O(5)–S–O(6) | 118·8 (2) | N–C(4)–C(1) | 121·9 (3) |
| C(1)–O(2)–C(5) | 116·4 (3) | O(2)–C(5)–C(6) | 108·1 (4) |
| C(2)–O(4)–C(7) | 116·8 (4) | O(4)–C(7)–C(8) | 107·8 (5) |
| C(12)–O(7)–C(15) | 117·9 (3) | C(10)–C(9)–C(14) | 118·7 (4) |
| S–N–C(4) | 118·7 (3) | S–C(9)–C(14) | 120·3 (3) |
| S–N–C(3) | 116·6 (3) | S–C(9)–C(10) | 120·9 (3) |
| C(3)–N–C(4) | 59·9 (2) | C(11)–C(10)–C(9) | 120·9 (4) |
| O(1)–C(1)–O(2) | 126·1 (4) | C(10)–C(11)–C(12) | 120·3 (4) |
| O(2)–C(1)–C(4) | 108·5 (4) | O(7)–C(12)–C(11) | 125·1 (4) |
| O(1)–C(1)–C(4) | 125·3 (4) | C(11)–C(12)–C(13) | 119·3 (4) |
| O(3)–C(2)–O(4) | 126·3 (4) | O(7)–C(12)–C(13) | 115·7 (4) |
| O(4)–C(2)–C(4) | 113·1 (4) | C(12)–C(13)–C(14) | 120·6 (4) |
| O(3)–C(2)–C(4) | 120·6 (4) | C(13)–C(14)–C(9) | 120·2 (4) |

| | |
|---|---|
| C(5)–O(2)–C(1)–O(1) | −5·4 (7) |
| C(1)–O(2)–C(5)–C(6) | −176·6 (4) |
| C(5)–O(2)–C(1)–C(4) | 176·2 (4) |
| C(7)–O(4)–C(2)–O(3) | 4·1 (7) |
| C(2)–O(4)–C(7)–C(8) | −163·6 (4) |
| C(7)–O(4)–C(2)–C(4) | −175·6 (4) |
| C(15)–O(7)–C(12)–C(11) | 2·1 (6) |
| C(15)–O(7)–C(12)–C(13) | −177·2 (4) |
| S–N–C(4)–C(1) | −2·1 (5) |
| S–N–C(4)–C(2) | −144·2 (3) |
| S–C(9)–C(10)–C(11) | 177·4 (4) |
| S–C(9)–C(14)–C(13) | −177·6 (4) |

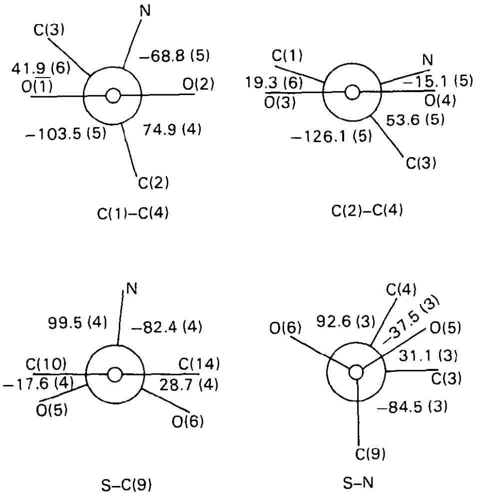

Fig. 2. Newman projections along the bonds C(1)–C(4), C(2)–C(4), S–C(9) and S–N. (Angles in deg.)

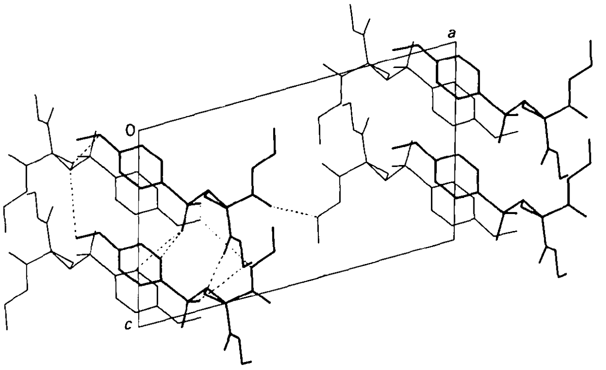

Fig. 3. Crystal packing projected along the *b* axis.

Table 3. *Shortest intermolecular distances*

| $A\cdots H–B$ | $A\cdots B$(Å) | $A\cdots$H(Å) | $\angle A\cdots H–B$(°) | Symmetry operation for *B* |
|---|---|---|---|---|
| O(1)···H(2)–C(3) | 3·475 (5) | 2·59 (3) | 147 (2) | $x, -\frac{1}{2}-y, \frac{1}{2}+z$ |
| O(3)···H(1)–C(7) | 3·554 (7) | 2·78 (4) | 138 (2) | $1-x, -y, 1-z$ |
| O(4)···H–C(15) | 3·521 (5) | 2·46 (1) | 167 (1) | $-x, -y, -z$ |
| O(5)···H–C(10) | 3·349 (6) | 2·80 (4) | 119 (2) | $-x, -y, 1-z$ |
| O(5)···H–C(14) | 3·334 (5) | 2·71 (3) | 125 (3) | $x, \frac{1}{2}-y, \frac{1}{2}+z$ |
| O(6)···H–C(15) | 3·468 (5) | 2·47 (1) | 154 (1) | $-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| O(6)···H(2)–C(5) | 3·377 (7) | 2·66 (4) | 126 (3) | $x, \frac{1}{2}-y, z-\frac{1}{2}$ |
| O(7)···H(1)–C(3) | 3·343 (5) | 2·62 (3) | 129 (2) | $-x, \frac{1}{2}+y, \frac{1}{2}-z$ |
| N···H–C(15) | 3·456 (6) | 2·73 (1) | 124·5 (4) | $-x, -y, -z$ |

All O,N···H distances ≤ 2·80 Å are included.

1978) in the orientation of the two methoxycarbonyl substituents with respect to the three-membered ring. The geometry around the C(1) and C(2) atoms is comparable with that of similar groups.

Crystal packing (Fig. 3) is governed by an extended short-distance network of the type C–H···O. These contacts, observed also in 1-methyl and 1-phenyl compounds, appear to be a significant factor in determining the conformation and the molecular packing in many organic crystal structures (Taylor & Kennard, 1982; Allen, Kennard & Taylor, 1983; Berkovitch-Yellin & Lieserowitz, 1984). Table 3 reports the geometry of the most relevant of these intermolecular interactions.

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*Acta Cryst.* (1985). C**41**, 222–224

# Structure of 1,3-Dimethyl-1,2,3,4,5,6-hexahydro-1,5-methano-3-benzazocin-9-ol Hydrobromide, $C_{14}H_{20}NO^+.Br^-$

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**Abstract.** $M_r = 298·23$, orthorhombic, $P2_12_12_1$, $a = 12·371\ (5)$, $b = 14·394\ (6)$, $c = 7·571\ (3)$ Å, $V = 1348\ (1)$ Å$^3$, $Z = 4$, $D_x = 1·467$ Mg m$^{-3}$, $\lambda(\text{Cu}\ K\alpha) = 1·5402$ Å, $\mu = 4·04$ mm$^{-1}$, $F(000) = 616$, $T = 293$ K, $R = 0·032$ for 1512 observed reflections. The title compound is a synthetic analgesic whose activity is as strong as codeine. The N-containing ring makes a right angle with the plane of the remaining part of the molecule. The H atom at the cationic N atom, which is shifted to the next position in the *C* ring in benzomorphan, is oriented towards the benezene ring. The distance between the N atom and the center of the benzene ring is 4·11 Å.

**Introduction.** In the course of our search for better analgesics, a number of attempts have been made to modify the morphine structure. Among them, the 6,7-benzomorphan structure has been one of the most promising starting points for the design of strong analgesics with insignificant abuse potentials, because selective ligands to these receptors were most likely to be found in the 6,7-benzomorphan series (Gilbert & Martin, 1976). Belleau, Conway, Ahmed & Hardy (1974) proposed that some geometrical requirements should be satisfied for the spatial orientation of the N lone-electron pair and the benzene ring. Opheim & Cox (1976) and Schiller, Yam & Lis (1977) suggested that the cationic form of the opiate drug is active and interacts with the receptors *via* ionic association; they therefore suggested that the distance from the cationic N atom to the benzene ring is critical for opiate–receptor interaction. In order to elucidate the structure–activity relationships and to verify the proposals described above, several modified benzomorphans, such as those with the *C* ring enlarged or with the N atom shifted to the next position in the *C* ring, were synthesized and their activities tested (Shiotani, Kometani, Mitsuhashi, Nozawa, Kurobe & Futsukaichi, 1976; Shiotani, Kometani & Mitsuhashi, 1975). All these compounds were shown to possess fairly strong analgesic activities (Shiotani, Kometani, Iitaka & Itai, 1978). The chemical structure of the title compound (1) (and the atomic numbering) is shown in Fig. 1, together with those of 2,9β-dimethyl-6,7-benzomorphan (2) and morphine (3).

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