

Fig. 1. The conformation of the molecule (2*S*-enantiomer depicted). The F atom is disordered between positions 2 and 6 of the phenyl ring (80,20% occupancy respectively).

essentially coplanar. It is likely that this 'W' conformation minimizes steric interactions between the three most bulky functional groups in the molecule, namely the *tert*-butyl, halophenyl and triazolyl groups. The triazolyl and halophenyl rings are also arranged to minimize intramolecular interactions, being inclined at angles of 85.5 (10) and 57.8 (10)° respectively to the plane containing C atoms C(31), C(4), C(5), C(6) and C(71) and at an angle of 55.3 (10)° to each other. The triazolyl ring is orientated such that C(1) and H(5) are almost eclipsed, the torsion angle C(1)—N(1)—C(5)—H(5) being 8.4 (11)°.

All four C—N distances and the N—N distance in the heterocyclic ring are intermediate between the expected single-bond lengths (1.47 and 1.45 Å respectively) and double-bond lengths (1.265 and 1.2 Å respectively) and the three atoms bonded to N(1) are coplanar with it. These data indicate extensive delocalization in the triazolyl ring. The exocyclic angles at N(1) show

considerable asymmetry, C(5)—N(1)—C(1) being significantly larger than C(5)—N(1)—N(2), and, as previously noted (Branch & Nowell, 1985), this asymmetry appears to be characteristic of the triazolyl ring itself rather than due to the influence of any intra- or intermolecular interactions.

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Structure and Absolute Configuration of a Penam Derivative

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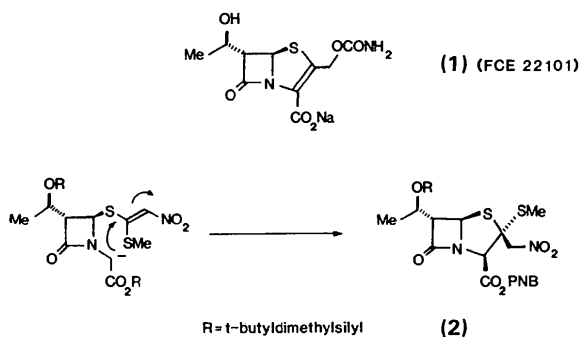
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Abstract. *p*-Nitrobenzyl 6-(1-*tert*-butyldimethylsiloxyethyl)-3-methylthio-3-nitromethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylate, C₂₃H₃₃N₃O₈S₂Si, *M_r* = 571.75, monoclinic, *P*2₁, *a* = 8.6734 (16), *b* = 10.420 (7), *c* = 16.785 (4) Å, β = 93.75 (2)°, *V* = 1513.7 Å³, *Z* = 2, *D_x* = 1.254 Mg m⁻³, λ(Cu Kα) =

1.54178 Å, μ = 2.33 mm⁻¹, *F*(000) = 604, *T* = 293 K, *R* = 0.061 for 1548 observed reflections. The absolute configuration was established. The main feature of this molecule is the bicyclic system related to that of penicillin. The five-membered ring, in the envelope conformation, shows a strong distortion when compared to carpetimycin or thienamycin. The four-membered ring is not planar and has torsion angles of ±10° as in the other two related compounds.

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Introduction. The β -lactam group of antibiotics continues to offer veritable challenges in chemistry, biology and medicine. The discovery of thienamycin (Albers-Schönberg, Arison, Kaczka, Kahan, Kahan, Lago, Maiese, Rhodes & Smith, 1976; Kahan, Kahan, Goegelman, Currie, Jackson, Stapley, Miller, Hendlin, Mochales, Hernandez & Woodruff, 1976), one of a potent class of novel β -lactams possessing unique structural and functional features, has fostered many new efforts in the synthesis of related types (Kametani, 1982; Ratcliffe & Albers-Schönberg, 1982). Concurrently, the pioneering work of the late R. B. Woodward (1977, 1978) and his coworkers (Ernest, Gosteli, Greengrass, Holick, Jackman, Pfandler & Woodward, 1978) has led to the synthesis of an unsaturated penicillin nucleus called penem. Combining the functional features of the carbapenems such as thienamycin, with the Woodward penam structure led intuitively to a 'hybrid penem', exemplified by expression (1) (FCE 22101) (Franceschi, Foglio, Alpegiani, Battistini, Bedeschi, Perrone, Zarini, Arcamone, Della Bruna & San Filippo, 1983) (Scheme 1). Several approaches and syntheses of this and related penems have been reported recently (Battistini, Scarafile, Foglio & Franceschi, 1984; Perrone, Alpegiani, Bedeschi, Giudici & Franceschi, 1984; Afonso, Hon, Weinstein, Ganguly & McPhail, 1982). Our synthesis of (1) (Hanessian, Bedeschi, Battistini & Mongelli, 1985) represented a tactically and operationally novel approach in which one of the crucial steps involved an intramolecular Michael reaction to produce the chiral bicyclic derivative (2). Interestingly, not only had this cyclization taken place with high stereoselection, but the seemingly more sterically demanding isomer had been formed as was evidenced from the X-ray analysis.



Scheme 1

Further studies in which kinetic and thermodynamic criteria can be considered must follow. On the other hand, stereoelectronic factors dealing with the dithioacetal-type functionality may have a bearing on the course of the asymmetric Michael cyclization. These features are under investigation.

Experimental. Recrystallization from a diisopropyl ether solution, m.p. 376–378 K, crystal size $0.04 \times 0.20 \times 0.50$ mm, unit-cell dimensions from 25 well centered reflections, $13 \leq 2\theta \leq 45^\circ$, Nonius CAD-4 diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, ω - 2θ scan, $\Delta\omega = (1.00 + 0.14 \tan\theta)^\circ$, $2\theta_{\max} = 140.0^\circ$ ($0 \leq h \leq 10$, $0 \leq k \leq 12$, $-20 \leq l \leq 20$), orientation monitored every 100 measurements, intensity checked every hour using three standard reflections (largest intensity fluctuation 1.2%). 3049 reflections measured of which 1548 with $I \geq 1.96\sigma(I)$ retained for structure determination and refinement. Lp correction, no absorption correction, direct methods (*MULTAN*)* block-diagonal least squares based on F , anisotropic for all non-H atoms, H atoms found on difference Fourier synthesis, H atoms held at a fixed distance, 0.95 Å, from their respective C atoms and given an isotropic temperature factor of 6.0 Å^2 ($B = 8.0 \text{ Å}^2$ for methyl H atoms). Function minimized $\sum w(|F_o| - |F_c|)^2$. Final $R = 0.061$, $wR = 0.066$ and $S = 1.97$ using weights derived from counting statistics. Maximum $(\Delta/\sigma) = 0.40$, average $(\Delta/\sigma) = 0.12$, electron density fluctuation on final difference Fourier synthesis -0.21 and $+0.28 \text{ e Å}^{-3}$. The real and imaginary parts of the anomalous dispersion for Si and S were included in the structure-factor calculation. The absolute configuration which was thus established corresponds to the set atomic coordinates presented in Table 1 since for the antipode of structure (2) the above indicators take the values of $R = 0.062$, $wR = 0.068$ and $S = 2.01$. Scattering curves for non-H atoms from Cromer & Mann (1968), those for H from Stewart, Davidson & Simpson (1965). Anomalous-dispersion coefficients f' and f'' for Si and S given by Cromer & Liberman (1970).

Discussion. The atomic numbering of the penam derivative is shown in Fig. 1 while a stereoscopic view of the molecule is presented in Fig. 2. The bond distances and angles calculated from the final refined coordinates are given in Table 2.†

The β -lactam ring system

Here the C(2)–C(3) bond is of the $C(sp^3)$ – $C(sp^3)$ type rather than the double bond observed in car-

* The programs used here are modified versions of *NRC-2*, data reduction, *NRC-10*, bond distances and angles, *NRC-22*, mean planes (Ahmed, Hall, Pippy & Huber, 1973), *FORDAP*, Fourier and Patterson maps (A. Zalkin), *MULTAN78*, multisolution program (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *NUCLS*, least-squares refinement (Doedens & Ibers, 1967) and *ORTEP*, stereodrawings (Johnson, 1965).

† Lists of structure factors, H-atom coordinates and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42589 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

petimycin A *p*-bromobenzyl ester (Nakayama, Kimura, Tanabe, Mizoguchi, Watanabe, Mori, Miyahara & Kawasaki, 1981) or in the *N*-acetylthienamycin methyl ester (Albers-Schönberg, Arison, Hensens, Hirshfield, Hoogsteen, Kaczka, Rhodes, Kahan, Kahan, Ratcliffe, Walton, Ruswinckle, Morin & Christensen, 1978). The conformation of this bicyclic system is characterized by the torsion angles listed in Table 2. The five-membered ring has the envelope conformation, folded along C(2)–C(5). The fold angle, *i.e.* the dihedral angle between plane 1 [S(1), C(2), C(5)] and plane 2 [C(2), C(3), N(4), C(5)], is 38.6°. The presence of the double bond between C(2) and C(3) leads to nearly planar five-membered rings in the two related compounds: carpetimycin (Nakayama *et al.*, 1981) and thienamycin (Albers-Schönberg *et al.*, 1978). The distortion of the β -lactam ring system is measured by the sum of the three N-atom bond angles ($\sum N$) and the distance (D) of the N atom from the plane of the attached three C atoms. Our measurements of the ring deformation, $\sum N = 338.3^\circ$ and $D = 0.39 \text{ \AA}$, reveal a less severe distortion of the β -lactam, when compared to the values of 326.3° , 0.51 \AA and 325.9° , 0.49 \AA in carpetimycin and thienamycin respectively.

In terms of bond distances and angles, the four-membered ring is comparable to those found in

carpetimycin and thienamycin. The same systematic effects are found. For example, the two intracyclic angles at N(4) and C(7) are larger, by at least 4° , than the other two angles. Also, the C=O bond has always the same asymmetric orientation, as measured by the angles N(4)–C(7)–O(1) = $130.6(9)^\circ$ and C(6)–C(7)–O(1) = $137.2(9)^\circ$. The atoms of the four-membered ring are not coplanar since all four torsion angles (Table 2) are significantly different from 0° . In a least-squares-plane calculation, assuming all four atoms to be coplanar, one finds deviations of up to $\pm 0.08(1) \text{ \AA}$ from that plane (plane 3). The two rings are fused and the dihedral angle (plane 2)/(plane 3) is 39° .

The substituents

The *tert*-butyldimethylsilyl group makes an α -junction at C(6) of the β -lactam as in the case of the *N*-acetylthienamycin methyl ester. However, in carpetimycin A *p*-bromobenzyl ester, the substituent at

Table 1. Final atomic coordinates for $C_{23}H_{33}N_3O_8S_2Si$ ($\times 10^4$) and $U_{eq} (\text{\AA}^2 \times 10^3)$

$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq}
S(1)	6632 (3)	9999	1103 (1)	68
S(2)	4101 (3)	11225 (3)	2022 (2)	76
Si	7593 (4)	6335 (4)	4014 (2)	93
O(1)	5784 (7)	6066 (6)	1541 (4)	87
O(2)	7792 (7)	7403 (7)	3302 (3)	68
O(3)	2434 (7)	7030 (6)	1270 (3)	68
O(4)	3745 (7)	7727 (6)	252 (3)	67
O(5)	1363 (7)	9961 (8)	758 (4)	88
O(6)	1582 (8)	11667 (8)	85 (5)	112
O(7)	–1358 (13)	1480 (11)	2687 (6)	193
O(8)	107 (14)	2114 (11)	3596 (5)	204
N(2)	2123 (9)	10733 (9)	437 (5)	82
N(3)	–381 (12)	2139 (10)	2923 (6)	118
N(4)	5447 (8)	8207 (7)	1938 (4)	55
C(2)	4542 (9)	10115 (10)	1229 (5)	64
C(3)	4032 (9)	8764 (9)	1527 (5)	54
C(5)	6863 (9)	9001 (10)	1975 (5)	59
C(6)	7811 (11)	7735 (10)	1917 (5)	65
C(7)	6247 (10)	7095 (10)	1735 (5)	66
C(8)	8767 (11)	7331 (10)	2667 (5)	67
C(9)	10164 (12)	8142 (14)	2830 (7)	105
C(10)	6693 (20)	5861 (14)	3560 (9)	163
C(11)	9485 (18)	5979 (19)	4499 (6)	162
C(12)	6306 (13)	7139 (13)	4685 (6)	99
C(13)	6989 (17)	8381 (14)	4951 (8)	131
C(14)	6067 (18)	6371 (21)	5449 (8)	167
C(15)	4732 (15)	7388 (18)	4251 (10)	157
C(16)	1969 (11)	5882 (10)	824 (6)	78
C(17)	1371 (9)	4919 (10)	1414 (5)	60
C(18)	273 (12)	4027 (12)	1113 (6)	84
C(19)	–293 (12)	3139 (11)	1624 (7)	91
C(20)	246 (11)	3096 (10)	2384 (6)	76
C(21)	1334 (12)	3965 (11)	2687 (6)	85
C(22)	1878 (11)	4855 (10)	2187 (5)	73
C(23)	5012 (14)	12690 (11)	1728 (8)	108
C(24)	3835 (10)	10537 (10)	415 (5)	70
C(25)	3385 (9)	7791 (10)	912 (5)	56

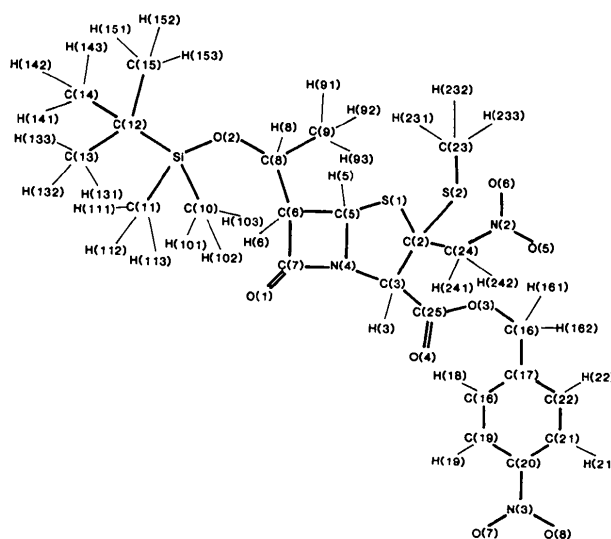


Fig. 1. Atomic numbering selected for the penam derivative (2).

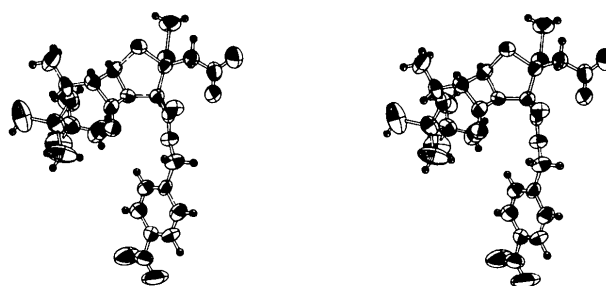


Fig. 2. Stereopair for the penam derivative (2).

C(6) was in the β orientation. The torsion angles C(5)–C(6)–C(8)–O(2), C(6)–C(8)–O(2)–Si, C(8)–O(2)–Si–C(12), O(2)–Si–C(12)–C(13), O(2)–Si–C(12)–C(14) and O(2)–Si–C(12)–C(15), which describe the conformation of the side chain as one progresses from C(5) to C(15), have values of 48.6 (6), 134.5 (6), 174.0 (6), –56.3 (8), –174.5 (8) and 63.5 (8)°, respectively.

The *p*-nitrobenzyl group of atoms is nearly planar, although there is a slight tilt, by 3.5° around N(3)–C(20), of the nitro group with respect to the phenyl plane of atoms.

Table 2. Bond distances (Å), angles (°) and torsion angles (°) of interest and their *e.s.d.*'s

S(1)–C(2)	1.843 (9)	C(12)–C(13)	1.480 (19)
S(1)–C(5)	1.796 (9)	C(12)–C(14)	1.537 (20)
S(2)–C(2)	1.823 (10)	C(12)–C(15)	1.527 (18)
S(2)–C(23)	1.803 (12)	N(2)–O(5)	1.191 (11)
Si(1)–O(2)	1.650 (7)	N(2)–O(6)	1.217 (12)
Si(1)–C(10)	1.863 (16)	N(2)–C(24)	1.502 (12)
Si(1)–C(11)	1.822 (15)	N(3)–O(7)	1.141 (15)
Si(1)–C(12)	1.839 (12)	N(3)–O(8)	1.180 (14)
C(2)–C(3)	1.567 (14)	N(3)–C(20)	1.474 (14)
C(2)–C(24)	1.525 (13)	C(16)–C(17)	1.524 (14)
C(3)–N(4)	1.486 (11)	C(17)–C(18)	1.401 (14)
C(3)–C(25)	1.527 (13)	C(18)–C(19)	1.374 (16)
N(4)–C(5)	1.479 (11)	C(19)–C(20)	1.330 (15)
N(4)–C(7)	1.404 (12)	C(20)–C(21)	1.381 (15)
C(5)–C(6)	1.561 (14)	C(21)–C(22)	1.356 (15)
C(6)–C(7)	1.524 (13)	C(22)–C(17)	1.344 (12)
C(6)–C(8)	1.521 (13)	C(25)–O(3)	1.317 (11)
C(7)–O(1)	1.183 (12)	C(25)–O(4)	1.172 (10)
C(8)–O(2)	1.405 (11)	O(3)–C(16)	1.454 (12)
C(2)–S(1)–C(5)	90.2 (4)	S(1)–C(2)–S(2)	112.4 (5)
S(1)–C(5)–N(4)	104.0 (6)	S(1)–C(2)–C(24)	104.9 (6)
C(5)–N(4)–C(3)	117.4 (7)	C(3)–C(2)–S(2)	105.1 (6)
N(4)–C(3)–C(2)	104.9 (7)	C(3)–C(2)–C(24)	116.1 (8)
C(3)–C(2)–S(1)	106.1 (6)	S(2)–C(2)–C(24)	112.3 (7)
N(4)–C(5)–C(6)	87.9 (6)	C(2)–S(2)–C(25)	102.8 (5)
C(5)–C(6)–C(7)	85.2 (7)	C(2)–C(24)–N(2)	110.9 (8)
C(6)–C(7)–N(4)	92.2 (7)	C(24)–N(2)–O(5)	119.8 (8)
C(7)–N(4)–C(5)	92.9 (7)	C(24)–N(2)–O(6)	116.6 (8)
C(3)–N(4)–C(7)	128.0 (7)	O(5)–N(2)–O(6)	123.6 (9)
S(1)–C(5)–C(6)	118.0 (6)	C(2)–C(3)–C(25)	118.7 (7)
N(4)–C(7)–O(1)	130.6 (9)	N(4)–C(3)–C(25)	108.1 (7)
C(6)–C(7)–O(1)	137.2 (9)	C(3)–C(25)–O(3)	107.7 (7)
C(5)–C(6)–C(8)	116.3 (8)	C(3)–C(25)–O(4)	124.6 (8)
C(7)–C(6)–C(8)	118.3 (8)	O(3)–C(25)–O(4)	127.6 (8)
C(6)–C(8)–O(2)	106.9 (7)	C(25)–O(3)–C(16)	114.9 (7)
C(6)–C(8)–C(9)	112.9 (8)	O(3)–C(16)–C(17)	107.6 (7)
O(2)–C(8)–C(9)	110.7 (8)	C(16)–C(17)–C(18)	117.0 (8)
C(8)–O(2)–Si(1)	127.6 (6)	C(16)–C(17)–C(22)	123.8 (8)
O(2)–Si(1)–C(10)	108.7 (6)	C(18)–C(17)–C(22)	119.1 (9)
O(2)–Si(1)–C(11)	109.1 (6)	C(17)–C(18)–C(19)	118.9 (10)
O(2)–Si(1)–C(12)	103.5 (6)	C(18)–C(19)–C(20)	120.3 (10)
C(10)–Si(1)–C(11)	110.8 (7)	C(19)–C(20)–C(21)	121.3 (10)
C(10)–Si(1)–C(12)	111.8 (6)	C(20)–C(21)–C(22)	118.5 (10)
C(11)–Si(1)–C(12)	112.6 (6)	C(21)–C(22)–C(17)	121.8 (9)
Si(1)–C(12)–C(13)	109.6 (9)	C(19)–C(20)–N(3)	119.4 (10)
Si(1)–C(12)–C(14)	113.2 (9)	C(21)–C(20)–N(3)	119.2 (9)
Si(1)–C(12)–C(15)	110.2 (9)	C(20)–N(3)–O(7)	119.3 (10)
C(13)–C(12)–C(14)	106.0 (11)	C(20)–N(3)–O(8)	118.6 (10)
C(13)–C(12)–C(15)	108.9 (11)	O(7)–N(3)–O(8)	122.0 (12)
C(14)–C(12)–C(15)	108.8 (11)		
S(1)–C(2)–C(3)–N(4)	26.2 (5)	C(5)–S(1)–C(2)–S(2)	76.8 (4)
C(2)–C(3)–N(4)–C(5)	0.9 (6)	C(5)–S(1)–C(2)–C(24)	–160.9 (5)
C(3)–N(4)–C(5)–S(1)	–28.1 (5)	N(4)–C(3)–C(2)–S(2)	–93.0 (4)
N(4)–C(5)–S(1)–C(2)	36.5 (5)	N(4)–C(3)–C(2)–C(24)	142.3 (7)
C(5)–S(1)–C(2)–C(3)	–37.9 (5)	S(1)–C(2)–C(3)–C(25)	–94.5 (6)
N(4)–C(5)–C(6)–C(7)	9.6 (6)	C(5)–N(4)–C(3)–C(25)	128.4 (8)
C(5)–C(6)–C(7)–N(4)	–10.1 (6)	C(3)–N(4)–C(7)–O(1)	–44.1 (6)
C(6)–C(7)–N(4)–C(5)	10.7 (6)	C(5)–C(6)–C(7)–O(1)	173.6 (6)
C(7)–N(4)–C(5)–C(6)	–10.4 (6)	S(1)–C(5)–C(6)–C(8)	145.5 (5)
		N(4)–C(7)–C(6)–C(8)	107.3 (3)

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