

Data collection

Siemens R3m/V diffractometer	$R_{int} = 0.0096$
$\theta/2\theta$ scans	$\theta_{max} = 25.08^\circ$
Absorption correction: none	$h = 0 \rightarrow 8$
1810 measured reflections	$k = 0 \rightarrow 12$
1621 independent reflections	$l = -13 \rightarrow 13$
971 observed reflections	3 standard reflections
$[I > 2\sigma(I)]$	monitored every 97 reflections
	linear decay of 2.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.6288P]$
$R(F) = 0.0547$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.1526$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.032$	$\Delta\rho_{max} = 0.265 \text{ e } \text{\AA}^{-3}$
1621 reflections	$\Delta\rho_{min} = -0.247 \text{ e } \text{\AA}^{-3}$
136 parameters	Atomic scattering factors
H atoms riding; C—H 0.96	from <i>International Tables for Crystallography</i> (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
for CH ₃ and 0.97 Å for CH ₂	

Table 3. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (II)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	U_{eq}
C1	0.7650 (4)	0.2613 (3)	0.9270 (3)	0.0447 (9)
C1A	0.8368 (5)	0.3875 (4)	0.8975 (4)	0.0623 (12)
N2	0.5676 (4)	0.2505 (3)	0.9352 (3)	0.0454 (8)
N2A	0.4702 (5)	0.3219 (3)	1.0147 (3)	0.0563 (9)
O2A	0.5631 (4)	0.3823 (3)	1.0819 (3)	0.0736 (9)
O2B	0.3043 (4)	0.3205 (3)	1.0058 (3)	0.0845 (11)
C3	0.4966 (5)	0.1355 (3)	0.8996 (3)	0.0448 (9)
O3	0.3492 (3)	0.0934 (3)	0.9163 (2)	0.0589 (8)
N4	0.6466 (4)	0.0810 (3)	0.8447 (3)	0.0424 (7)
N4A	0.6488 (5)	-0.0473 (3)	0.8245 (3)	0.0525 (8)
O4A	0.5023 (4)	-0.1002 (3)	0.8158 (3)	0.0711 (9)
O4B	0.7999 (4)	-0.0925 (3)	0.8167 (3)	0.0736 (9)
C5	0.8185 (5)	0.1468 (3)	0.8617 (3)	0.0435 (9)
C5A	0.9476 (5)	0.1506 (4)	0.7617 (4)	0.0644 (12)
C6	0.8759 (5)	0.1623 (3)	0.9871 (3)	0.0481 (9)

Table 4. Selected geometric parameters (\AA , $^\circ$) for (II)

C1—N2	1.452 (4)	C3—O3	1.189 (4)
C1—C6	1.504 (5)	C3—N4	1.407 (4)
C1—C1A	1.506 (5)	N4—N4A	1.409 (4)
C1—C5	1.507 (5)	N4—C5	1.454 (4)
N2—N2A	1.405 (4)	N4A—O4B	1.213 (4)
N2—C3	1.406 (5)	N4A—O4A	1.216 (4)
N2A—O2A	1.210 (4)	C5—C5A	1.506 (5)
N2A—O2B	1.214 (4)	C5—C6	1.506 (5)
N2—C1—C6	116.0 (3)	N4—C5—C6	113.9 (3)
N2—C1—C1A	116.1 (3)	C5A—C5—C6	124.5 (3)
C6—C1—C1A	124.3 (3)	N4—C5—C1	103.7 (3)
N2—C1—C5	103.6 (3)	C5A—C5—C1	122.3 (3)
C6—C1—C5	60.0 (2)	C6—C5—C1	59.9 (2)
C1A—C1—C5	122.6 (3)	C1—C6—C5	60.1 (2)
N4—C5—C5A	117.7 (3)		

For both compounds, data collection: *SHELXTL-Plus* (Sheldrick, 1991); cell refinement: *SHELXTL-Plus*; data reduction: *SHELXTL-Plus*; program(s) used to solve structures: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1098). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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7-Benzyl-3-thia-7-azabicyclo[3.3.1]nonane 3-Oxide

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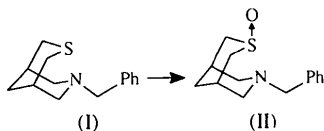
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Abstract

The molecular geometry of a major metabolite, C₁₄H₁₉NOS, of a potent anti-arrhythmic drug, 7-benzyl-3-thia-7-azabicyclo[3.3.1]nonane (BRB-I-28), has been determined by X-ray diffraction. The 3,7-dihetero bicyclic system of the sulfoxide molecule adopts a chair-chair conformation like that of the HClO₄ salt of the BRB-I-28 molecule. The S...N contact distance of 2.863 (2) Å in the present molecule is significantly shorter than that found in the crystal structure of its precursor [3.038 (4) Å]. The overall molecule possesses pseudo-mirror symmetry.

Comment

Several members of the family of 3,7-dihetero bicyclo[3.3.1]nonanes have demonstrated significant anti-arrhythmic activity in dog models (Bailey *et al.*, 1984; Scherlag, Patterson, Lazzara, Bailey, Thompson & Berlin, 1988; Fazekas, Mabo, Berlin, Scherlag & Lazzara, 1992) and in myocardial tissues (Patterson, Scherlag, Berlin & Lazzara, 1991, 1993). The title compound, 7-benzyl-3-thia-7-azabicyclo[3.3.1]nonane 3-oxide, (II), is the major metabolite of a potent anti-arrhythmic drug 7-benzyl-3-thia-7-azabicyclo[3.3.1]nonane perchlorate, *i.e.* (I).HClO₄ (Chen *et al.*, 1995), and the first to be identified from an ensemble of the family of 3,7-dihetero bicyclo[3.3.1]nonanes. The crystal structure of the metabolite was determined in order to confirm the structure and to see the effect of S-oxidation on the conformation of the molecule.



The 3,7-dihetero bicyclo[3.3.1]nonane portion of the sulfoxide molecule (II) assumes a chair-chair (CC) conformation, with a very short S···N contact distance of 2.863 (2) Å (Fig. 1). The perchlorate salt of the precursor molecule (I) has been shown (Bailey *et al.*, 1984) to adopt a CC conformation also, but with a significantly longer S···N contact distance of 3.038 (4) Å. In the latter compound, the N(7) atom is protonated and the molecular conformation is stabilized by an intramolecular N(7)—H···S hydrogen bond. In at least two other related compounds, namely, 7-benzyl-3-thia-7-azabicyclo[3.3.1]nonane-9,9-diol (Bailey, Berlin & Holt, 1984) and 7-benzyl-9-phenyl-3-thia-7-azabicyclo[3.3.1]nonan-9-ol (Bailey *et al.*, 1984), N(7) protonation led to N—H···S hydrogen bonding, with N···S distances of 2.991 (3) and 3.047 (3) Å, respectively, for the above mentioned compounds. A much longer S···N distance of 3.100 (2) Å has been reported for a related tricyclic system, 3,6-dibenzyl-8a-methoxy-5H-4a,8-(methanothiomethano)-2H-hexahydropyrido[3,4-*e*]-1,3-oxazine (Smith, Berlin, Zisman, Holt, Green & van der Helm, 1988), where the N atom is a free amine, as in the present structure, but the S atom is unsubstituted. It seems that oxidation of the S atom in the present structure reduces the orbital repulsion, which leads to a shorter S···N contact. The ring torsion angles C(1)—C(8)—N(7)—C(6) of -61.6 (2) and C(5)—C(6)—N(7)—C(8) of 62.0 (2)° indicate that the shorter S···N distance is achieved through puckering of the nitrogen end of the piperidine ring. In all the related structures referred to above, the piperidine ring is slightly flattened.

The oxidation of the S atom has virtually no effect on the two C—S distances [1.821 (2) and 1.820 (2) Å],

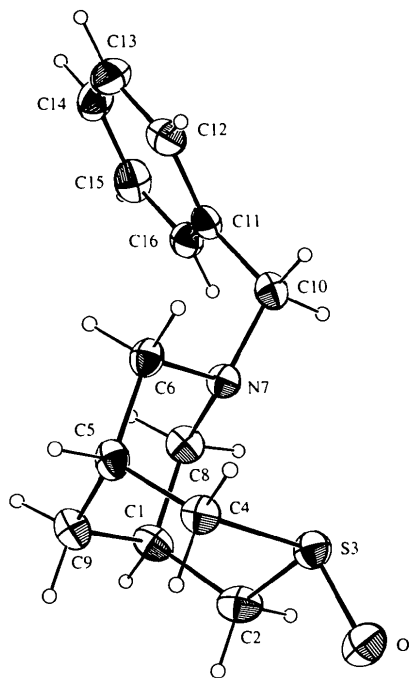


Fig. 1. A perspective ORTEP drawing (Johnson, 1965) of compound (II) with 50% probability ellipsoids shown for the non-H atoms.

which are comparable to the corresponding distances [range 1.819 (3)–1.831 (4) Å] found in the four related compounds involving an unsubstituted S atom (Bailey *et al.*, 1984; Bailey, Holt & Berlin, 1984; Smith *et al.*, 1988). The C—S—C angle of 96.9 (1)° in the present structure is, however, significantly smaller than that observed [99.3 (2)–100.9 (2)°] in the thiane ring of the four related structures. The C—H distances in the molecule range between 0.91 (2) and 1.00 (2) Å.

The phenyl ring assumes a nearly symmetrical position with respect to the bicyclic system, giving the overall molecule a pseudo-mirror symmetry. The S=O bond is inclined at an angle of 36° to the plane of the thiane ring and may be considered to be in a pseudo-equatorial position. Both the S=O distance [1.513 (1) Å] and the C—S—C angle [96.9 (1)°] are comparable with those [1.504 (2) Å and 95.1 (1)°] found in 4-acetyl-*trans*-3-methylcarbamoyl-1,4-thiazinane 1-oxide (Vanhouteghem, Lenstra, Giese, Van der Auwera & Anteunis, 1985), where the S=O group takes an inclined position.

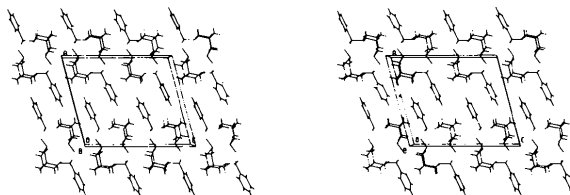


Fig. 2. A stereoview of the crystal packing viewed down the *b* axis.

Experimental

The title compound was crystallized from HCCl_3 /pentane by slow evaporation.

Crystal data

$\text{C}_{14}\text{H}_{19}\text{NOS}$

$M_r = 249.4$

Monoclinic

$P2_1/c$

$a = 13.084 (3) \text{ \AA}$

$b = 6.527 (1) \text{ \AA}$

$c = 15.397 (3) \text{ \AA}$

$\beta = 104.66 (2)^\circ$

$V = 1272.1 (7) \text{ \AA}^3$

$Z = 4$

$D_x = 1.302 \text{ Mg m}^{-3}$

D_m not measured

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 48 reflections

$\theta = 11-18^\circ$

$\mu = 0.19 \text{ mm}^{-1}$

$T = 138 \text{ K}$

Prismatic

$0.33 \times 0.26 \times 0.14 \text{ mm}$

Light yellow

Data collection

Enraf-Nonius CAD-4

diffractometer

$\omega/2\theta$ scans

Absorption correction: none

2740 measured reflections

2618 independent reflections

2073 observed reflections

$[I > 2\sigma(I)]$

$R_{\text{int}} = 0.02$

$\theta_{\text{max}} = 26.5^\circ$

$h = -16 \rightarrow 16$

$k = 0 \rightarrow 8$

$l = 0 \rightarrow 19$

3 standard reflections

frequency: 120 min

intensity decay: 3%

Refinement

Refinement on F

$R = 0.044$

$wR = 0.043$

$S = 1.9$

2073 reflections

230 parameters

All H-atom parameters

refined

$w = 1/\sigma^2(F)$

$(\Delta/\sigma)_{\text{max}} = 0.03$

$\Delta\rho_{\text{max}} = 0.42 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
C(1)	0.2781 (2)	0.7209 (4)	0.0768 (1)	0.0260 (7)
C(2)	0.3943 (2)	0.7604 (4)	0.0802 (2)	0.0292 (8)
S(3)	0.48947 (4)	0.58973 (9)	0.15183 (4)	0.0246 (2)
O(1)	0.5844 (1)	0.5950 (2)	0.1126 (1)	0.0325 (6)
C(4)	0.4221 (2)	0.3508 (3)	0.1116 (1)	0.0230 (7)
C(5)	0.3036 (2)	0.3456 (3)	0.1048 (1)	0.0234 (7)
C(6)	0.2784 (2)	0.3768 (3)	0.1956 (1)	0.0230 (7)
N(7)	0.3121 (1)	0.5825 (3)	0.2289 (1)	0.0208 (6)
C(8)	0.2551 (2)	0.7411 (4)	0.1687 (1)	0.0253 (7)
C(9)	0.2458 (2)	0.5075 (5)	0.0388 (2)	0.0274 (8)
C(10)	0.3099 (2)	0.6135 (4)	0.3234 (1)	0.0245 (7)
C(11)	0.2025 (2)	0.5980 (4)	0.3429 (1)	0.0235 (7)
C(12)	0.1682 (2)	0.4156 (4)	0.3732 (1)	0.0286 (8)
C(13)	0.0710 (2)	0.4032 (4)	0.3924 (2)	0.0364 (9)
C(14)	0.0049 (2)	0.5728 (4)	0.3811 (2)	0.0371 (9)
C(15)	0.0374 (2)	0.7545 (4)	0.3501 (2)	0.0341 (8)
C(16)	0.1352 (2)	0.7666 (4)	0.3314 (1)	0.0268 (8)

Table 2. Selected geometric parameters (\AA , $^\circ$)

C(1)—C(2)	1.530 (3)	C(8)—C(1)	1.525 (2)
S(3)—C(2)	1.820 (2)	C(9)—C(1)	1.528 (3)
S(3)—C(4)	1.821 (2)	C(10)—C(11)	1.512 (3)
N(7)—C(6)	1.465 (3)	C(11)—C(12)	1.395 (3)
N(7)—C(8)	1.462 (3)	C(12)—C(13)	1.379 (3)
N(7)—C(10)	1.476 (3)	C(13)—C(14)	1.389 (4)
S(3)—O(1)	1.513 (1)	C(14)—C(15)	1.385 (4)
C(4)—C(5)	1.529 (3)	C(15)—C(16)	1.383 (3)
C(5)—C(6)	1.530 (2)	C(16)—C(11)	1.393 (3)
C(5)—C(9)	1.527 (3)	S(3)···N(7)	2.863 (2)
C(2)—S(3)—C(4)	96.9 (1)	C(4)—C(5)—C(9)	110.7 (2)
O(1)—S(3)—C(2)	104.4 (1)	C(6)—C(5)—C(9)	109.3 (2)
O(1)—S(3)—C(4)	105.0 (1)	C(5)—C(6)—N(7)	109.1 (2)
C(6)—N(7)—C(8)	111.5 (2)	N(7)—C(8)—C(1)	109.8 (2)
C(6)—N(7)—C(10)	113.1 (2)	C(1)—C(9)—C(5)	109.5 (2)
C(8)—N(7)—C(10)	113.2 (2)	C(10)—C(11)—C(12)	121.2 (2)
N(7)—C(10)—C(11)	115.9 (2)	C(10)—C(11)—C(16)	120.8 (2)
C(2)—C(1)—C(8)	112.4 (2)	C(12)—C(11)—C(16)	118.0 (2)
C(2)—C(1)—C(9)	110.1 (2)	C(11)—C(12)—C(13)	121.0 (2)
C(8)—C(1)—C(9)	109.4 (2)	C(12)—C(13)—C(14)	120.4 (2)
C(1)—C(2)—S(3)	116.1 (2)	C(13)—C(14)—C(15)	119.3 (2)
S(3)—C(4)—C(5)	116.0 (1)	C(14)—C(15)—C(16)	120.1 (2)
C(4)—C(5)—C(6)	112.6 (2)	C(15)—C(16)—C(11)	121.1 (2)
C(1)—C(2)—S(3)—C(4)		47.7 (2)	
C(2)—S(3)—C(4)—C(5)		-47.1 (1)	
S(3)—C(4)—C(5)—C(9)		61.2 (2)	
C(4)—C(5)—C(9)—C(1)		-67.1 (2)	
C(5)—C(9)—C(1)—C(2)		67.3 (2)	
C(9)—C(1)—C(2)—S(3)		-62.0 (2)	
C(1)—C(9)—C(5)—C(6)		57.4 (2)	
C(9)—C(5)—C(6)—N(7)		-59.3 (2)	
C(6)—N(7)—C(10)—C(11)		-63.0 (2)	
C(1)—C(8)—N(7)—C(6)		-61.6 (2)	
C(8)—N(7)—C(6)—C(5)		62.0 (2)	
N(7)—C(6)—C(5)—C(9)		-59.3 (2)	
C(6)—C(5)—C(9)—C(1)		57.4 (2)	
C(5)—C(9)—C(1)—C(8)		-56.7 (2)	
C(9)—C(1)—C(8)—N(7)		58.1 (2)	
C(8)—C(7)—C(10)—C(11)		65.0 (2)	
N(7)—C(10)—C(11)—C(16)		-84.7 (2)	
N(7)—C(10)—C(11)—C(12)		95.6 (2)	

All H atoms were located from difference Fourier maps and refined with isotropic displacement parameters. The structure was determined by direct methods and refined by full-matrix least squares.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: local least-squares cell refinement program. Data reduction: local program. Program(s) used to solve structure: *MULTAN80* (Main *et al.*, 1980). Program(s) used to refine structure: *SHELX76* (Sheldrick, 1976). Molecular graphics: *ORTEP* (Johnson, 1965) and *PLUTO* (Motherwell & Clegg, 1978).

This work was supported by NIH grant No. CA17562 (DvdH).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1188). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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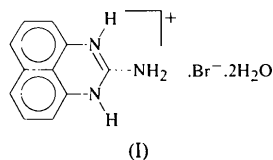
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Comment

It is known that 2-aminoperimidylammonium chloride is an excellent reagent for the removal of sulfate ions (Stephen, 1970). However, the synthesis of this compound is inconvenient, and the purification procedure described by Stephen (1970) does not remove every trace of sulfur-containing impurities from the product (McClure, 1973). A synthetic method for the preparation of the bromide salt, free of sulfate impurities, is given by McClure (1973) and is suggested to be a simpler preparation of the sulfate-removing reagent. For experimental purposes, it was desired by one of the authors (CEM) to prepare a polymer of this compound to remove sulfate from water. It was also desired that the polymer be easy to handle and reusable. Such a polymer was prepared, but it retained sulfate too strongly to be regenerated efficiently. Subsequent work on the polymer has provided a way to regenerate the polymer and will be reported at a future date.

The crystal structure of the title compound, (I), was determined by three-dimensional X-ray diffraction analysis in order to study possible sulfate binding sites. An unsuccessful attempt was made to complex the title compound with sulfate using a gel-permeation technique in order to determine exactly how and where the compound binds to sulfate.



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2-Aminoperimidinium Bromide Dihydrate

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Abstract

The title compound, C₁₁H₁₀N₃⁺.Br⁻.2H₂O, is essentially planar along the aminoperimidine skeleton, with an r.m.s. deviation of 0.009 Å and a maximum deviation of 0.017 Å. Due to the presence of two water molecules, extensive hydrogen bonding exists in the crystal. Hydrogen bonds *via* the two water molecules join the Br⁻ ion to both the amine N atom and one of the ring N atoms. The other ring N atom and the amine N atom also form hydrogen bonds to the Br⁻ ion from the second molecule in the unit cell.

The plane defined by all the non-H atoms in the aminoperimidine skeleton displayed a maximum deviation of 0.017 Å for atom N1 and an r.m.s. deviation of

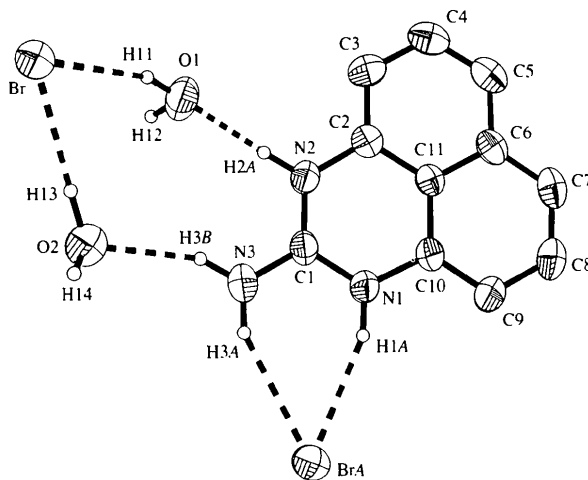


Fig. 1. View of the title compound. Displacement ellipsoids are shown at 50% probability levels and H atoms are drawn as small spheres of arbitrary radii.