confirmed by MS, IR and NMR spectra (Glinka, 1985). The compound shows neuroleptic activity (Glinka, 1986). Previous papers (Stępień, Wajsman, Grabowski, Glinka & Perrin, 1987; Olszak, Stępień, Wajsman, Grabowski, Glinka & Lecocq, 1987) give details of the properties and structure of related compounds.

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Crystal Studies of Heterocyclic Compounds Containing One Oxygen and Two Nitrogen Atoms. XVII. *N,N'*-Bis(tosyl)perhydro-1,5,7-oxadiazecine

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Abstract. $C_{27}H_{28}N_2O_5S_2$, $M_r = 452{\cdot}6$, orthorhombic, *Pnaa*, $a = 11{\cdot}814\ (2)$, $b = 18{\cdot}257\ (3)$, $c = 20{\cdot}683\ (3)$ Å, $V = 4461\ (1)$ Å^3, $Z = 8$, $D_m = 1{\cdot}327$, $D_x = 1{\cdot}348\ (1)$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 24{\cdot}1$ cm^{-1}, $F(000) = 1920$, room temperature, $R = 0{\cdot}0512$ for 3533 reflections with $I > 3\sigma(I)$. The ten-membered perhydrooxadiazecine ring is in a boat–chair–boat conformation. The ring is approximately symmetrical with respect to a pseudo-twofold axis; the asymmetry parameter [Duax & Norton (1975). *Atlas of Steroid Structure*, Vol. I. New York: IFI/Plenum] $\Delta_2 = 9{\cdot}9°$. Both tosyl groups are axial. The weighted least-squares planes of both benzene rings form an angle of 86·3 (1)°.

Experimental. This paper is a continuation of the study of the structure–biological-activity relationship of perhydrooxadiazecine derivatives that show neuroleptic activity.

Colourless, thick tabular crystals from ethanol at room temperature. D_m measured by flotation. The specimen used for for X-ray work, 0·2 × 0·2 × 0·3 mm, was cut from a larger crystal. Diffraction data measured on a CAD-4 diffractometer using θ–2θ scan technique, graphite-monochromatized Cu $K\alpha$ radiation. Unit-cell parameters obtained by least squares using setting angles of 22 reflections with $\theta_{max} = 40{\cdot}7°$. Data collected in range $2{\cdot}1 < \theta < 73{\cdot}1°$; not corrected for absorption; standard reflection 533, maximum change 9·9%; range of h, k and l: 0 to 14, 0 to 22, 0 to 25, respectively. Of 4244 independent reflections 3533 were considered observed by the criterion $I > 3\sigma(I)$ and used in calculations. Solution by direct methods using *SHELX*76 (Sheldrick, 1976), H atoms located from difference Fourier map, refinement by full-matrix least-squares procedure on F magnitudes, 383 parameters. Refinement to final $R = 0{\cdot}0512$, $S = 1{\cdot}546$, unit weights. Max. shift/e.s.d. = 0·57; largest peaks, 0·62 and 0·60 e Å^{-3}, on a final difference map near S atom (1·06 Å); the next peak is 0·45 e Å^{-3}. Scattering factors from *SHELX*76. The geometry of the

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Table 1. *Final fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$) *with e.s.d.'s in parentheses*

$$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	U_{eq}
S1	2429 (1)	1096 (0)	828 (0)	510 (2)
O1	2161 (2)	1688 (1)	411 (1)	665 (9)
O2	3141 (2)	1229 (2)	1378 (1)	674 (8)
C11	3019 (3)	380 (2)	374 (1)	506 (11)
C12	3640 (3)	−159 (2)	670 (2)	629 (13)
C13	3988 (3)	−753 (3)	322 (2)	743 (16)
C14	3708 (3)	−837 (2)	−334 (2)	689 (14)
C15	3114 (4)	−284 (3)	−619 (2)	693 (14)
C16	2762 (3)	322 (2)	−289 (2)	603 (12)
C141	4045 (7)	−1511 (4)	−706 (4)	1074 (29)
S2	−464 (1)	−486 (0)	2109 (0)	528 (2)
O3	−1498 (2)	−219 (1)	2387 (1)	765 (11)
O4	−505 (2)	−848 (1)	1497 (1)	683 (10)
C21	115 (3)	−1103 (2)	2673 (2)	504 (10)
C22	1236 (3)	−1094 (2)	2834 (2)	732 (16)
C23	1663 (4)	−1604 (3)	3255 (2)	788 (17)
C24	1016 (3)	−2141 (2)	3522 (2)	636 (13)
C25	−128 (4)	−2139 (2)	3362 (2)	763 (16)
C26	−571 (3)	−1629 (2)	2949 (2)	708 (14)
C241	1511 (7)	−2708 (4)	3974 (4)	979 (24)
N1	1221 (2)	776 (1)	1110 (1)	462 (8)
C2	320 (3)	642 (2)	616 (2)	558 (12)
C3	−335 (4)	1307 (3)	418 (2)	682 (15)
C4	−709 (4)	1762 (2)	983 (2)	695 (14)
O5	−1200 (2)	1292 (1)	1453 (1)	607 (8)
C6	−1131 (4)	1566 (2)	2098 (2)	669 (15)
C7	58 (4)	1501 (2)	2390 (2)	614 (13)
C8	420 (3)	744 (2)	2573 (2)	554 (11)
N9	391 (2)	198 (1)	2052 (1)	463 (8)
C10	1336 (3)	189 (2)	1589 (2)	491 (11)

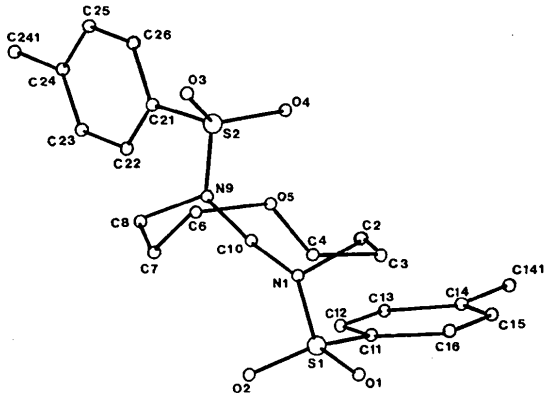

Fig. 1. The structure of the molecule with the atom-numbering scheme.

molecule was calculated using *CRYSRULER* (Rizzoli, Sangermano, Calestani & Andreetti, 1987). The positional parameters and equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1,* interatomic distances and angles in Table 2, and torsion angles in the oxadiazecine ring in Table 3. The molecular structure and the atom-numbering scheme are shown in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54347 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

S1—O1	1·419 (2)	S2—O3	1·435 (2)
S1—O2	1·435 (2)	S2—O4	1·429 (2)
S1—C11	1·754 (3)	S2—C21	1·760 (3)
S1—N1	1·648 (2)	S2—N9	1·610 (3)
C11—C12	1·372 (5)	C21—C22	1·366 (5)
C11—C16	1·409 (4)	C21—C26	1·380 (5)
C12—C13	1·365 (6)	C22—C23	1·371 (6)
C13—C14	1·405 (6)	C23—C24	1·361 (5)
C14—C15	1·364 (6)	C24—C25	1·391 (5)
C14—C141	1·505 (7)	C24—C241	1·511 (7)
C15—C16	1·365 (5)	C25—C26	1·368 (6)
N1—C2	1·495 (4)	O5—C6	1·427 (4)
N1—C10	1·467 (4)	C6—C7	1·534 (5)
C2—C3	1·498 (5)	C7—C8	1·496 (5)
C3—C4	1·500 (6)	C8—N9	1·469 (4)
C4—O5	1·420 (4)	N9—C10	1·470 (4)

C11—S1—N1	105·6 (1)	C21—S2—N9	107·5 (1)
O2—S1—N1	106·7 (1)	O4—S2—N9	108·3 (1)
O2—S1—C11	108·5 (2)	O4—S2—C21	107·7 (2)
O1—S1—N1	107·0 (1)	O3—S2—N9	107·5 (1)
O1—S1—C11	109·3 (2)	O3—S2—C21	106·4 (2)
O1—S1—O2	119·0 (2)	O3—S2—O4	118·9 (2)
S1—C11—C16	119·4 (3)	S2—C21—C26	119·4 (3)
S1—C11—C12	120·6 (3)	S2—C21—C22	122·1 (3)
C12—C11—C16	119·7 (3)	C22—C21—C26	118·5 (4)
C11—C12—C13	119·7 (4)	C21—C22—C23	120·2 (4)
C12—C13—C14	121·7 (4)	C22—C23—C24	122·7 (4)
C13—C14—C141	121·4 (5)	C23—C24—C241	121·8 (4)
C13—C14—C15	117·2 (4)	C23—C24—C25	116·6 (4)
C15—C14—C141	121·4 (5)	C25—C24—C241	121·7 (4)
C14—C15—C16	122·7 (4)	C24—C25—C26	121·5 (4)
C11—C16—C15	118·8 (4)	C21—C26—C25	120·5 (4)
S1—N1—C10	114·7 (2)	O5—C6—C7	113·2 (3)
S1—N1—C2	115·7 (2)	C6—C7—C8	115·6 (3)
C2—N1—C10	114·0 (3)	C7—C8—N9	115·8 (3)
N1—C2—C3	115·0 (3)	S2—N9—C8	119·1 (2)
C2—C3—C4	112·7 (3)	C8—N9—C10	117·9 (3)
C3—C4—O5	108·7 (3)	S2—N9—C10	121·0 (2)
C4—O5—C6	113·8 (3)	N1—C10—N9	111·2 (3)

Table 3. *Torsion angles* (°) *in the oxadiazecine ring*

S1—N1—C10—N9	149·8 (2)	S2—N9—C10—N1	117·8 (3)
S1—N1—C2—C3	−81·6 (4)	S2—N9—C8—C7	−115·9 (3)
N9—C10—N1—C2	−73·5 (3)	C4—O5—C6—C7	−75·1 (4)
C10—N1—C2—C3	142·2 (3)	O5—C6—C7—C8	−73·1 (4)
N1—C2—C3—C4	−46·3 (5)	C6—C7—C8—N9	56·6 (5)
C2—C3—C4—O5	−47·5 (5)	C7—C8—N9—C10	79·8 (4)
C3—C4—O5—C6	153·6 (3)	C8—N9—C10—N1	−78·3 (3)

Related literature. A previous paper (Stępień, Brzozowski, Grabowski, Krakowiak & Bavoux, 1988) gives details of the properties and structures of related compounds.

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