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8-Chloro-4a,14a-epoxy-1,2,3,4,5,14-hexahydrophthalazino[2,3-*b*]phthalazine-7,12-dione*

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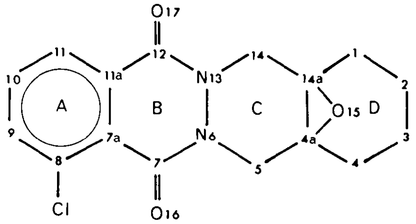
Abstract. $C_{16}H_{15}ClN_2O_3$, triclinic, $P\bar{1}$, $a = 14\cdot834$ (2), $b = 11\cdot231$ (1), $c = 8\cdot874$ (1) Å, $\alpha = 102\cdot74$ (1), $\beta = 78\cdot99$ (1), $\gamma = 88\cdot77$ (1)°, $Z = 4$, $D_x = 1\cdot50$ Mg m^{-3}, μ(Mo $K\alpha$) = 0·290 mm^{-1}. Final $R = 0\cdot060$. There are two independent molecules in the asymmetric unit which adopt different conformations. Considered as strips, both of them are twisted by about 17° on average.

Introduction. Previous work (Foces-Foces, Cano & García-Blanco, 1977*a*, 1978) described the structures of two three-ring epoxides. It seems feasible that different tetracycline analogues will be obtained when the epoxide ring is opened, because of its reactivity. Continuing with the project on the analogues of tetracyclines, we have determined the structure of the title compound (I).



(I)

A crystal 0·32 × 0·27 × 0·08 mm was used. The lattice parameters and intensities were measured on a PW 1100 four-circle diffractometer, with graphite-monochromated Mo $K\alpha$ radiation ($\omega/2\theta$ scan mode). 2841 reflexions with $I > 2\sigma(I)$ were considered as observed. Absorption effects were corrected with *ORABS* (Schwarzenbach, 1972) (range of trans-

Table 1. *Final positional parameters with their e.s.d.'s for the heavy atoms*

	Molecule (1)			Molecule (2)		
	x	y	z	x	y	z
Cl	0·5565 (1)	0·2925 (1)	0·9439 (2)	0·0780 (1)	0·2236 (1)	0·0619 (1)
C(1)	0·6031 (4)	−0·4476 (5)	0·2998 (8)	0·0958 (3)	−0·4568 (4)	−0·6793 (6)
C(2)	0·6904 (6)	−0·4754 (8)	0·1846 (9)	0·1852 (4)	−0·5356 (5)	−0·7066 (8)
C(3)	0·7685 (5)	−0·4172 (7)	0·2081 (11)	0·2676 (3)	−0·4603 (5)	−0·7297 (8)
C(4)	0·7656 (4)	−0·2925 (6)	0·3023 (7)	0·2712 (3)	−0·3616 (5)	−0·5851 (6)
C(4a)	0·6778 (3)	−0·2516 (4)	0·4203 (5)	0·1781 (3)	−0·2974 (4)	−0·5017 (5)
C(5)	0·6616 (3)	−0·1174 (4)	0·4828 (6)	0·1799 (3)	−0·1660 (4)	−0·4285 (6)
N(6)	0·5745 (2)	−0·0766 (3)	0·6015 (4)	0·0903 (2)	−0·1080 (3)	−0·3412 (4)
C(7)	0·5726 (3)	0·0333 (4)	0·7019 (5)	0·0902 (3)	−0·0031 (4)	−0·2283 (5)
C(7a)	0·4900 (3)	0·0683 (4)	0·8301 (5)	0·0027 (3)	0·0713 (4)	−0·1647 (5)
C(8)	0·4780 (3)	0·1790 (4)	0·9431 (5)	−0·0088 (3)	0·1735 (4)	−0·0382 (5)
C(9)	0·4013 (4)	0·2062 (5)	1·0639 (6)	−0·0931 (3)	0·2401 (5)	0·0160 (6)
C(10)	0·3334 (4)	0·1247 (5)	1·0712 (7)	−0·1665 (4)	0·2070 (5)	−0·0543 (6)
C(11)	0·3420 (3)	0·0165 (6)	0·9616 (6)	−0·1569 (3)	0·1091 (5)	−0·1812 (6)
C(11a)	0·4208 (3)	−0·0129 (4)	0·8424 (5)	−0·0729 (3)	0·0401 (4)	−0·2349 (5)
C(12)	0·4267 (3)	−0·1308 (4)	0·7276 (5)	−0·0671 (3)	−0·0671 (4)	−0·3643 (5)
N(13)	0·5029 (2)	−0·1579 (3)	0·6115 (4)	0·0138 (2)	−0·1363 (3)	−0·4148 (4)
C(14)	0·5055 (3)	−0·2643 (5)	0·4828 (7)	0·0108 (3)	−0·2560 (4)	−0·5203 (6)
C(14a)	0·5998 (3)	−0·3285 (4)	0·4198 (5)	0·0929 (3)	−0·3432 (4)	−0·5483 (5)
O(15)	0·6553 (2)	−0·3248 (3)	0·5376 (4)	0·1184 (2)	−0·3656 (3)	−0·4066 (3)
O(16)	0·6375 (3)	0·0975 (4)	0·6830 (4)	0·1633 (2)	0·0243 (3)	−0·1869 (4)
O(17)	0·3650 (3)	−0·2020 (3)	0·7331 (4)	−0·1330 (2)	−0·0997 (3)	−0·4269 (4)

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[*] Crystal and Molecular Structures of Diazapolycyclic Compounds. V.

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Table 2. *Final positional parameters with their e.s.d.'s and bond distances* (Å) *for the hydrogen atoms*

	Molecule (1)				Molecule (2)			
	x	*y*	*z*	H bond	*x*	*y*	*z*	H bond
H(1*a*)	0·595 (4)	−0·505 (6)	0·362 (7)	0·94 (8)	0·047 (4)	−0·507 (5)	−0·655 (6)	0·96 (6)
H(1*b*)	0·554 (7)	−0·451 (9)	0·254 (12)	0·90 (12)	0·097 (3)	−0·433 (4)	−0·779 (6)	0·98 (6)
H(2*a*)	0·698 (3)	−0·558 (5)	0·121 (6)	0·97 (5)	0·190 (4)	−0·601 (6)	−0·794 (7)	0·93 (6)
H(2*b*)	0·677 (3)	−0·465 (5)	0·080 (6)	1·02 (8)	0·182 (4)	−0·568 (5)	−0·610 (7)	1·00 (7)
H(3*a*)	0·821 (5)	−0·432 (6)	0·123 (8)	0·96 (7)	0·269 (4)	−0·428 (6)	−0·812 (8)	0·88 (8)
H(3*b*)	0·808 (5)	−0·470 (6)	0·253 (8)	1·02 (8)	0·323 (5)	−0·514 (6)	−0·764 (8)	0·97 (6)
H(4*a*)	0·779 (6)	−0·244 (7)	0·243 (10)	0·90 (10)	0·312 (4)	−0·303 (6)	−0·612 (7)	0·94 (7)
H(4*b*)	0·815 (6)	−0·271 (7)	0·351 (9)	0·93 (9)	0·293 (4)	−0·401 (5)	−0·510 (6)	0·97 (6)
H(5*a*)	0·654 (3)	−0·083 (4)	0·390 (6)	1·01 (6)	0·206 (3)	−0·128 (4)	−0·513 (6)	0·97 (5)
H(5*b*)	0·704 (4)	−0·082 (5)	0·540 (7)	0·92 (6)	0·218 (3)	−0·161 (4)	−0·355 (5)	0·93 (5)
H(9)	0·395 (5)	0·279 (5)	1·136 (6)	0·91 (5)	−0·094 (4)	0·306 (5)	0·097 (7)	0·91 (5)
H(10)	0·292 (4)	0·136 (5)	1·156 (7)	0·86 (6)	−0·227 (6)	0·260 (7)	−0·022 (9)	1·02 (8)
H(11)	0·302 (4)	−0·042 (5)	0·969 (6)	0·90 (6)	−0·205 (4)	0·088 (5)	−0·232 (7)	0·93 (7)
H(14*a*)	0·483 (4)	−0·244 (5)	0·397 (7)	0·96 (7)	0·011 (3)	−0·241 (4)	−0·618 (6)	0·92 (6)
H(14*b*)	0·466 (4)	−0·313 (5)	0·536 (6)	0·94 (6)	−0·038 (3)	−0·292 (4)	−0·480 (5)	0·89 (5)

Table 3. *Bond lengths* (Å) *and angles* (°)

	(1)	(2)		(1)	(2)		(1)	(2)
C(1)–C(2)	1·468 (10)	1·527 (7)	N(6)–C(7)	1·350 (5)	1·367 (5)	C(10)–C(11)	1·365 (7)	1·373 (6)
C(1)–C(14a)	1·508 (7)	1·518 (6)	N(6)–N(13)	1·417 (5)	1·422 (5)	C(11)–C(11a)	1·397 (6)	1·396 (6)
C(2)–C(3)	1·371 (12)	1·508 (8)	C(7)–C(7a)	1·484 (5)	1·472 (5)	C(11a)–C(12)	1·472 (6)	1·457 (6)
C(3)–C(4)	1·460 (9)	1·510 (7)	C(7)–O(16)	1·223 (5)	1·233 (5)	C(12)–N(13)	1·354 (5)	1·360 (5)
C(4)–C(4a)	1·498 (6)	1·520 (6)	C(7a)–C(8)	1·399 (6)	1·399 (5)	C(12)–O(17)	1·229 (5)	1·237 (6)
C(4a)–C(5)	1·485 (6)	1·478 (6)	C(7a)–C(11a)	1·392 (6)	1·398 (6)	N(13)–C(14)	1·454 (6)	1·465 (5)
C(4a)–C(14a)	1·459 (6)	1·471 (6)	C(8)–Cl	1·744 (5)	1·735 (5)	C(14)–C(14a)	1·507 (6)	1·494 (6)
C(4a)–O(15)	1·458 (6)	1·453 (5)	C(8)–C(9)	1·383 (6)	1·388 (6)	C(14a)–O(15)	1·444 (6)	1·450 (6)
C(5)–N(6)	1·494 (5)	1·463 (5)	C(9)–C(10)	1·378 (8)	1·374 (8)			

C(2)–C(1)–C(14a)	113·6 (6)	111·2 (4)	N(6)–C(7)–C(7a)	116·6 (4)	117·8 (4)	C(7a)–C(11a)–C(12)	121·2 (3)	121·1 (4)
C(1)–C(2)–C(3)	122·5 (7)	110·8 (4)	N(6)–C(7)–O(16)	119·3 (3)	118·4 (3)	C(11a)–C(12)–N(13)	117·2 (4)	118·1 (4)
C(2)–C(3)–C(4)	122·4 (6)	112·7 (5)	C(7a)–C(7)–O(16)	124·1 (4)	123·8 (4)	C(11a)–C(12)–O(17)	122·3 (4)	123·1 (4)
C(3)–C(4)–C(4a)	114·6 (5)	113·8 (4)	C(7)–C(7a)–C(8)	123·3 (4)	123·4 (4)	N(13)–C(12)–O(17)	120·5 (4)	118·7 (4)
C(4)–C(4a)–C(5)	115·3 (4)	115·1 (4)	C(7)–C(7a)–C(11a)	119·3 (3)	118·8 (3)	C(12)–N(13)–N(6)	121·5 (3)	121·4 (3)
C(4)–C(4a)–C(14a)	119·9 (4)	120·8 (3)	C(8)–C(7a)–C(11a)	117·4 (4)	117·8 (4)	C(12)–N(13)–C(14)	118·9 (4)	116·0 (4)
C(4)–C(4a)–O(15)	115·1 (4)	115·4 (4)	C(7a)–C(8)–Cl	123·7 (3)	123·4 (3)	C(14)–N(13)–N(6)	119·1 (3)	121·0 (3)
C(5)–C(4a)–C(14a)	119·8 (3)	119·0 (4)	C(7a)–C(8)–C(9)	121·4 (4)	120·6 (4)	N(13)–C(14)–C(14a)	113·6 (4)	116·3 (4)
C(5)–C(4a)–O(15)	115·1 (3)	114·9 (3)	C(9)–C(8)–Cl	114·9 (4)	116·0 (3)	C(14)–C(14a)–C(1)	115·1 (4)	115·2 (4)
C(14a)–C(4a)–O(15)	59·3 (3)	59·5 (3)	C(10)–C(9)–C(8)	119·7 (5)	120·5 (4)	C(14)–C(14a)–C(4a)	116·7 (4)	119·2 (4)
C(4a)–C(5)–N(6)	115·3 (4)	114·0 (3)	C(11)–C(10)–C(9)	120·5 (5)	120·4 (5)	C(14)–C(14a)–O(15)	114·2 (4)	114·9 (3)
C(5)–N(6)–C(7)	116·6 (3)	117·1 (3)	C(10)–C(11)–C(11a)	119·9 (5)	119·6 (5)	C(1)–C(14a)–C(4a)	122·0 (4)	120·9 (3)
C(5)–N(6)–N(13)	119·1 (3)	116·7 (3)	C(11)–C(11a)–C(7a)	121·1 (4)	121·1 (4)	C(1)–C(14a)–O(15)	117·1 (4)	114·7 (4)
C(7)–N(6)–N(13)	124·1 (3)	122·2 (3)	C(11)–C(11a)–C(12)	117·7 (4)	117·8 (4)	C(4a)–C(14a)–O(15)	60·3 (3)	59·6 (3)
						C(14a)–O(15)–C(4a)	60·4 (3)	60·9 (3)

Table 4. *Torsion angles* (°)

	(1)	(2)	Ring *C*	(1)	(2)
O(17)–C(12)–N(13)–C(14)	7·7 (6)	−10·8 (5)	φ_0 = C(5)–N(6)–N(13)–C(14)	−15·7 (5)	31·3 (5)
C(11a)–C(12)–N(13)–C(14)	−170·9 (4)	167·4 (4)	φ_1 = N(6)–N(13)–C(14)–C(14a)	42·3 (6)	−1·7 (5)
O(17)–C(12)–N(13)–N(6)	179·2 (4)	−176·2 (3)	φ_2 = N(13)–C(14)–C(14a)–C(4a)	−34·1 (5)	−13·9 (4)
C(5)–N(6)–C(7)–O(16)	6·1 (5)	−12·9 (5)	φ_3 = C(14)–C(14a)–C(4a)–C(5)	0·8 (6)	0·0 (4)
C(5)–N(6)–C(7)–C(7a)	−173·9 (4)	166·5 (4)	φ_4 = C(14a)–C(4a)–C(5)–N(6)	25·7 (5)	28·5 (5)
N(13)–N(6)–C(7)–O(16)	−179·5 (4)	−169·4 (3)	φ_5 = C(4a)–C(5)–N(6)–N(13)	−18·6 (5)	−44·1 (4)
Ring *B*	(1)	(2)	Ring *D*	(1)	(2)
C(12)–N(13)–N(6)–C(7)	−1·4 (6)	−7·5 (5)	φ_0 = C(4)–C(4a)–C(14a)–C(1)	−2·1 (7)	1·1 (5)
N(13)–N(6)–C(7)–C(7a)	0·5 (6)	10·0 (5)	φ_1 = C(4a)–C(14a)–C(1)–C(2)	−1·2 (8)	20·7 (5)
N(6)–C(7)–C(7a)–C(11a)	1·2 (6)	−7·5 (5)	φ_2 = C(14a)–C(1)–C(2)–C(3)	16·2 (11)	−51·8 (5)
C(7)–C(7a)–C(11a)–C(12)	−2·0 (6)	2·5 (5)	φ_3 = C(1)–C(2)–C(3)–C(4)	−28·7 (11)	63·6 (5)
C(7a)–C(11a)–C(12)–N(13)	1·1 (6)	0·2 (5)	φ_4 = C(2)–C(3)–C(4)–C(4a)	23·2 (8)	−40·0 (5)
C(11a)–C(12)–N(13)–N(6)	0·5 (5)	2·0 (4)	φ_5 = C(3)–C(4)–C(4a)–C(14a)	−7·8 (7)	8·3 (5)

mission factor: 0·93–0·98). Lorentz and polarization corrections were applied.

The structure was solved with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977). All heavy atoms were located from an *E* map calculated with the set of phases having the highest combined figure of merit. There are two crystallographically independent molecules in the asymmetric unit.

Least-squares calculations refined the structure to give the H atoms in a difference synthesis. They were included in the final refinement with isotropic thermal factors; the non-hydrogen atoms were treated anisotropically. The weighting scheme was chosen to give no trends in $\langle w\Delta^2\rangle$ over ranges of F_o and $\sin\theta/\lambda$. The final $R = 0{\cdot}060$ and $R_w = 0{\cdot}069$.

A final difference synthesis had no significant peaks, the residual electron density being no greater than $\pm 0{\cdot}39$ e Å^{-3}.

Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Coordinates for the heavy atoms are listed in Table 1 and for the H atoms in Table 2, together with their bond distances. Table 3 shows the bond lengths and angles.*

Discussion. Both molecules were tested by half-normal probability plots (Abrahams & Keve, 1971) (Fig. 1), comparing homologous intramolecular distances. The main differences are in the length of C(2)–C(3) and the conformations of rings *C* and *D*. In Table 4, the torsion angles of rings *B*, *C* and *D* are given. The parameters describing the conformations of rings *C* and *D* are listed in Table 5 (Cano, Foces-Foces & Garcia-Blanco, 1977). According to these values, the conformations are: in molecule (1), ring *C* is almost halfway between boat (0,3) and diplanar (3,5) and ring *D* is an envelope distorted towards diplanar (1,5). In molecule (2), ring *C* is almost diplanar (1,3) while ring *D* is halfway between envelope (0,5) and half-chair (0) (Bucourt & Haitnaut, 1965).

The mean angles around N(6) and N(13) for molecules (1) and (2) are (119·9; 119·8°) and (118·7; 119·5°) respectively. The distortion parameters (Winkler & Dunitz, 1971) about C(12)–N(13) and N(6)–C(7) are greater at N than at C, as usual (Table 5).

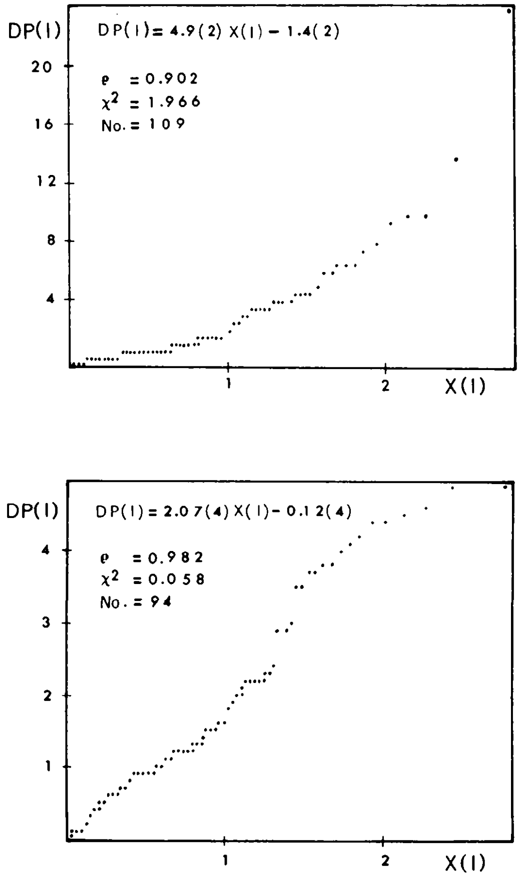

Fig. 1. Half-normal probability plots.

Table 5. *Conformational parameters* (°)

(*a*) Distortion parameters for N(13) and N(6)

	N(13)		N(6)	
	(1)	(2)	(1)	(2)
χ_N	−8·5 (7)	14·6 (6)	−5·6 (6)	23·5 (6)
χ_C	1·4 (7)	−1·8 (6)	0·0 (5)	−0·6 (6)
τ	−175·9 (3)	175·6 (3)	−176·7 (3)	178·6 (3)

(*b*) Parameters for rings *C* and *D* [φ_0 is the torsion angle around N(6)–N(13) and C(4a)–C(14a)]

	Ring *C*		Ring *D*	
	(1)	(2)	(1)	(2)
τ_m	−8·1 (5)	15·3 (5)	12·5 (9)	−30·6 (5)
q	35·6 (3)	29·1 (3)	15·9 (5)	33·1 (4)
Σ	204 (1)	114 (1)	331 (4)	24 (1)
δ	206 (2)	116 (2)	76 (11)	315 (6)
α_1	205 (1)	115 (1)	203 (6)	169 (3)
α_2	−1 (1)	0 (1)	127 (6)	−145 (3)

(*c*) Parameters for the 'strip' description

Plane	θ		φ		τ		κ	
	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
Ring *A*	0	0	–	–	90	90	0	0
Ring *B*	0	3	136	77	90	89	0	3
Ring *C*	17	16	111	49	96	80	15	12
Ring *D*	11	17	153	−3	99	173	5	271

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34222 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 6. *Some least-squares planes through the atoms marked with an asterisk*

The atomic deviations are in Å.

Ring *A*	(1)	(2)	Ring *B*	(1)	(2)	Ring *C*	(1)	(2)	Ring *D*	(1)	(2)
C(7a)*	0·000 (5)	−0·004 (5)	N(6)*	0·007 (4)	−0·044 (3)	C(4a)*	0·122 (5)	0·051 (4)	C(1)*	−0·014 (6)	0·167 (3)
C(8)*	−0·011 (5)	0·006 (5)	C(7)*	0·002 (5)	0·046 (5)	C(5)*	−0·203 (5)	−0·222 (5)	C(2)*	0·108 (9)	−0·349 (6)
C(9)*	0·011 (6)	0·001 (6)	C(7a)*	−0·010 (5)	−0·020 (4)	N(6)*	0·055 (4)	0·227 (3)	C(3)*	−0·135 (9)	0·292 (6)
C(10)*	−0·001 (6)	−0·011 (6)	C(11a)*	0·010 (5)	−0·007 (5)	N(13)*	0·186 (4)	−0·055 (4)	C(4)*	0·066 (6)	−0·064 (6)
C(11)*	−0·010 (6)	0·013 (6)	C(12)*	−0·001 (5)	0·012 (5)	C(14)*	−0·266 (6)	−0·109 (5)	C(4a)*	0·018 (5)	−0·084 (5)
C(11a)*	0·010 (5)	−0·005 (5)	N(13)*	−0·007 (4)	0·013 (4)	C(14a)*	0·106 (5)	0·108 (4)	C(14a)*	−0·043 (5)	0·038 (5)
Cl	−0·055 (2)	0·002 (1)	O(16)	0·006 (4)	0·190 (4)				O(15)	−1·236 (4)	−1·253 (3)
			O(17)	−0·029 (4)	−0·011 (4)						

The geometries of the epoxide rings, as far as their areas are concerned, agree with those reported elsewhere (Foces-Foces, Cano & García-Blanco, 1977*a*). In the present work, $A_1 = 0{\cdot}915$ and $A_2 = 0{\cdot}920$ Å^2.

Some least-squares planes are given in Table 6. The Cl atoms do not deviate, within the limits of error, from their respective benzene rings [0·055 for molecule (1) and 0·002 Å for molecule (2)]. The atoms in the diazaquinone rings are coplanar, including the attached O atoms.

The molecules considered as strips can be described with reference to intrinsic orthonormal axes $\{T,N,B\}$ (Foces-Foces, Cano & García-Blanco, 1977*b*), with the unit normal taken as that to the aromatic rings on each molecule and *B* towards the Cl atom in the aromatic plane. The parameters θ reflect the angular separation of the normal characterizing each ring, to give an idea of the overall twist, about 17° from end to end in both molecules (Table 5).

No significant intermolecular distances <4 Å were found.

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Structure de l'Isopropyl-1 {[(Chloro-3 phénylthio)-4 pyridyl-3]sulfonyl}-3 Urée

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Abstract. $C_{15}H_{16}ClN_3O_3S_2$, monoclinic, $P2_1/a$, a = 21·079 (5), b = 8·813 (3), c = 10·008 (3) Å, β = 106·18 (2)°, V = 1785·5 Å^3, Z = 4, D_x = 1·435 Mg m^{-3}, μ(Cu $K\alpha$) = 4·155 mm^{-1}. The structure was refined to an R of 0·055 for 2430 unique diffractometer data. Comparison with the molecules of torasemide confirms that there is no correlation between the conformation of the $-SO_2-NH-CO-$ group and the deprotonation of N atoms which occurs in three of the four molecules of torasemide. The conformation is not determined by the stacking of the molecules in the crystal.

Introduction. Dans le cadre de l'étude de composés diurétiques ayant des actions supposées analogues, nous avons récemment publié les structures de deux

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