(Saheki, Yamada, Yoshioka & Nakatsu, 1976; Maverick, Trueblood & Bekoe, 1978), and trinitrofluorenone (Brown, Cheung, Trefonas & Majeste, 1974).

I thank Dr Robert Battershell of the Diamond-Shamrock Corp. for a gift of the trichlorotricyanobenzene.

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Structure of 2-Benzyl-2,3-dihydro-3-oxo-4-piperidino-1,2,5-thiazole 1,2-Dioxide

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(*Received* 9 *May* 1988; *accepted* 1 *August* 1988)

Abstract. $C_{14}H_{17}N_3O_3S$, $M_r = 307{\cdot}37$, triclinic, $P\bar{1}$, $a = 16{\cdot}3875\ (7)$, $b = 10{\cdot}9715\ (3)$, $c = 9{\cdot}0822\ (3)$ Å, $\alpha = 105{\cdot}757\ (3)$, $\beta = 99{\cdot}465\ (3)$, $\gamma = 72{\cdot}412\ (3)°$, $U = 1492{\cdot}1\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}37$ Mg m^{-3}, graphite-monochromated Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $\mu = 2{\cdot}009$ mm^{-1}, $F(000) = 648$, $T = 293$ K, $R = 0{\cdot}076$ for 2654 observed reflexions [$I > 3\sigma(I)$]. Bond lengths and angles in molecules *A* and *B* are within 2·5 times the pooled e.s.d.'s. The main difference between the molecules is the conformation of the phenyl rings with respect to the thiazole ring. The N(1) and N(3) atoms are sp^2 hybridized: sums of angles are 359·6 (7), 359·4 (6)° (molecule *A*) and 359·7 (7), 359·9 (8)° (molecule *B*). The piperidine ring exhibits a chair conformation.

Experimental. Colourless plate, 0·30 × 0·20 × 0·03 mm, used for data collection and determination of lattice constants (Cu $K\alpha$, 78 reflexions with $2 < \theta < 45°$). Philips PW 1100 diffractometer, Cu $K\alpha$, graphite monochromator, bisecting geometry, $\omega/2\theta$ scan mode, 5062 independent reflexions up to $\theta = 65°$, *hkl* range −18,18; −12,12; 0,10. Two standard reflexions were measured every 90 min, no decay observed, but the diffraction was rather weak, with only about 50% of the 5062 total recorded reflexions observed. The structure was solved by direct methods (*MULTAN*80, Main *et al.*, 1980). H atoms, located in a difference synthesis, included isotropically in last cycles of refinement. Empirical weights so as to give no trends in $\langle w\Delta F^2 \rangle$ *versus* $\langle |F_o| \rangle$ and $\langle (\sin\theta)/\lambda \rangle$ [ΔF was adjusted by

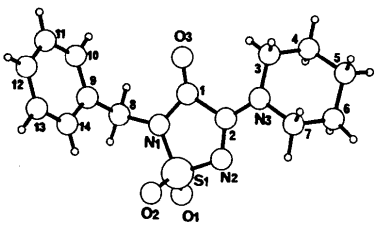

Fig. 1. A view of one of the two nearly identical molecules projected on the molecular least-squares plane showing the atomic numbering.

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Table 1. *Final atomic coordinates and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$) *for* $C_{14}H_{17}O_3N_3S$

$$U_{eq} = \tfrac{1}{3}\sum U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j \cos(\mathbf{a}_i,\mathbf{a}_j).$$

	x	y	z	U_{eq}
S(1*A*)	0·4731 (1)	0·1614 (2)	0·2014 (2)	462 (8)
O(1*A*)	0·4444 (3)	0·1637 (5)	0·0456 (6)	646 (24)
O(2*A*)	0·4529 (3)	0·2858 (5)	0·3081 (6)	605 (23)
O(3*A*)	0·6731 (3)	−0·0902 (5)	0·2733 (6)	602 (24)
N(1*A*)	0·5791 (4)	0·0950 (6)	0·2153 (6)	503 (26)
N(2*A*)	0·4477 (4)	0·0503 (6)	0·2552 (7)	516 (26)
N(3*A*)	0·5124 (4)	−0·1488 (6)	0·3184 (7)	498 (26)
C(1*A*)	0·6019 (5)	−0·0231 (7)	0·2562 (8)	461 (31)
C(2*A*)	0·5151 (4)	−0·0440 (7)	0·2762 (8)	439 (29)
C(3*A*)	0·5828 (6)	−0·2663 (8)	0·3260 (11)	608 (41)
C(4*A*)	0·5625 (7)	−0·3847 (10)	0·2173 (12)	754 (47)
C(5*A*)	0·4768 (7)	−0·3999 (11)	0·2438 (15)	829 (54)
C(6*A*)	0·4062 (7)	−0·2769 (11)	0·2359 (12)	768 (53)
C(7*A*)	0·4272 (6)	−0·1574 (10)	0·3458 (12)	667 (44)
C(8*A*)	0·6439 (6)	0·1459 (10)	0·1710 (9)	601 (39)
C(9*A*)	0·6947 (5)	0·2069 (8)	0·3090 (9)	559 (37)
C(10*A*)	0·7802 (6)	0·1455 (11)	0·3408 (12)	685 (45)
C(11*A*)	0·8278 (7)	0·2041 (13)	0·4682 (13)	798 (56)
C(12*A*)	0·7904 (8)	0·3228 (13)	0·5568 (15)	823 (59)
C(13*A*)	0·7063 (8)	0·3870 (11)	0·5290 (13)	830 (53)
C(14*A*)	0·6584 (5)	0·3295 (9)	0·4023 (12)	698 (42)
S(1*B*)	0·9828 (1)	0·1283 (2)	0·8449 (2)	508 (8)
O(1*B*)	1·0559 (3)	0·0923 (6)	0·9477 (7)	746 (27)
O(2*B*)	0·9790 (4)	0·2336 (6)	0·7776 (6)	683 (26)
O(3*B*)	0·7762 (3)	0·0901 (6)	0·9097 (6)	690 (26)
N(1*B*)	0·8938 (4)	0·1645 (6)	0·9344 (7)	512 (26)
N(2*B*)	0·9643 (4)	0·0050 (6)	0·7173 (7)	571 (28)
N(3*B*)	0·8572 (4)	−0·1028 (7)	0·6324 (8)	604 (30)
C(1*B*)	0·8437 (5)	0·0848 (8)	0·8694 (9)	525 (33)
C(2*B*)	0·8901 (5)	−0·0140 (8)	0·7314 (9)	541 (33)
C(3*B*)	0·7807 (6)	−0·1393 (10)	0·6467 (13)	698 (45)
C(4*B*)	0·8058 (8)	−0·2833 (11)	0·6498 (15)	913 (59)
C(5*B*)	0·8511 (10)	−0·3708 (12)	0·5076 (19)	1027 (68)
C(6*B*)	0·9305 (7)	−0·3235 (11)	0·5008 (15)	865 (53)
C(7*B*)	0·9014 (8)	−0·1841 (10)	0·4959 (14)	803 (52)
C(8*B*)	0·8822 (7)	0·2637 (9)	1·0838 (11)	704 (46)
C(9*B*)	0·8472 (5)	0·4016 (8)	1·0617 (8)	517 (33)
C(10*B*)	0·7625 (6)	0·4481 (10)	1·0088 (12)	743 (46)
C(11*B*)	0·7328 (9)	0·5725 (12)	0·9870 (15)	973 (63)
C(12*B*)	0·7817 (12)	0·6537 (12)	1·0146 (15)	1010 (69)
C(13*B*)	0·8656 (12)	0·6141 (14)	1·0669 (14)	1060 (75)
C(14*B*)	0·8983 (8)	0·4855 (13)	1·0883 (13)	898 (58)

Table 2. *Selected geometrical parameters* (Å, °) *for molecules A and B*

	A	*B*		*A*	*B*
S(1)–O(1)	1·420 (5)	1·417 (6)	S(1)–O(2)	1·423 (5)	1·427 (7)
S(1)–N(1)	1·667 (6)	1·677 (7)	N(1)–C(1)	1·371 (11)	1·334 (11)
C(1)–C(2)	1·553 (12)	1·550 (10)	C(2)–N(2)	1·294 (8)	1·326 (11)
N(2)–S(1)	1·611 (8)	1·596 (6)	C(2)–N(3)	1·321 (11)	1·316 (10)
N(1)–C(8)	1·491 (13)	1·490 (10)	C(8)–C(9)	1·501 (11)	1·504 (13)
N(3)–C(3)	1·456 (10)	1·461 (14)	C(3)–C(4)	1·493 (13)	1·515 (17)
C(4)–C(5)	1·527 (19)	1·534 (19)	C(5)–C(6)	1·499 (14)	1·554 (22)
C(6)–C(7)	1·511 (15)	1·469 (17)	C(7)–N(3)	1·493 (13)	1·471 (13)
C(1)–O(3)	1·188 (8)	1·201 (11)			

O(1)–S(1)–O(2)	115·3 (3)	116·5 (3)	O(1)–S(1)–N(1)	108·8 (3)	109·1 (3)
O(1)–S(1)–N(2)	112·8 (3)	112·6 (4)	O(2)–S(1)–N(1)	109·3 (3)	109·3 (4)
O(2)–S(1)–N(2)	112·3 (3)	111·1 (4)	N(1)–S(1)–N(2)	96·7 (3)	96·2 (3)
S(1)–N(1)–C(1)	112·7 (5)	113·2 (5)	N(1)–C(1)–C(2)	104·4 (6)	105·9 (7)
C(1)–C(2)–N(2)	115·2 (7)	113·2 (7)	C(2)–N(2)–S(1)	110·9 (5)	111·5 (6)
N(1)–C(1)–O(3)	125·9 (8)	126·7 (8)	C(2)–C(1)–O(3)	129·7 (7)	127·5 (8)
C(1)–C(2)–N(3)	121·3 (7)	123·6 (7)	N(2)–C(2)–N(3)	123·4 (7)	123·0 (7)
C(2)–N(3)–C(3)	127·0 (7)	126·7 (8)	C(2)–N(3)–C(7)	118·2 (7)	120·2 (8)
C(3)–N(3)–C(7)	114·5 (7)	113·0 (8)	S(1)–N(1)–C(8)	125·4 (6)	120·7 (6)
C(1)–N(1)–C(8)	121·5 (7)	125·5 (6)	N(1)–C(8)–C(9)	111·7 (7)	111·8 (7)

	A	*B*
N(3)–C(3)–C(4)–C(5)	−54·2 (11)	−56·1 (13)
C(3)–C(4)–C(5)–C(6)	54·7 (13)	56·8 (14)
C(4)–C(5)–C(6)–C(7)	−54·7 (13)	−57·8 (14)
C(5)–C(6)–C(7)–N(3)	53·9 (12)	59·6 (13)
C(6)–C(7)–N(3)–C(3)	−55·0 (10)	−60·7 (12)
C(7)–N(3)–C(3)–C(4)	55·4 (10)	57·0 (11)
C(1)–C(2)–N(3)–C(3)	−11·4 (12)	−10·8 (13)
C(1)–N(1)–C(8)–C(9)	−79·2 (9)	−105·8 (9)
N(1)–C(8)–C(9)–C(10)	109·8 (10)	73·5 (11)
N(1)–C(1)–C(2)–N(2)	−1·8 (9)	1·0 (9)
C(1)–C(2)–N(2)–S(1)	4·0 (8)	−1·8 (9)
C(2)–N(2)–S(1)–N(1)	−4·0 (6)	1·7 (6)
N(2)–S(1)–N(1)–C(1)	2·9 (6)	−1·1 (6)
S(1)–N(1)–C(1)–C(2)	−1·1 (7)	0·3 (8)

least squares to a linear model dependent on F_o and then $w\Delta F$ fitted to a linear model on $(\sin\theta)/\lambda$] (Martínez-Ripoll, Cano, García-Blanco, Martínez-Carrera & Gundel, 1977). $R = 0.076$, $wR = 0.073$, $S = 1.09$. Max. and average $\Delta/\sigma = 0.90$ and 0·12. Final $\Delta\rho = \pm 0.35$ e Å^{-3}. No extinction correction. Computing with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) on a VAX 11/750 computer. Scattering factors from *International Tables for X-ray Crystallography* (1974). Final atomic coordinates for the non-H atoms and the main geometrical parameters are given in Tables 1 and 2,* according to the numbering scheme given in Fig. 1 (*PLUTO*, Motherwell & Clegg, 1978).

* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles, torsion angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51328 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. The synthesis of the title compound has recently been published (compound 5g, Aran, Ruiz & Stud, 1987).

We thank Dr V. Aran for suggesting the problem and providing the material.

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