1192 reflections
173 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F)$

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

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

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

	x	y	z	U_{eq}
(I)				
O1	0.4181 (1)	−0.1493 (1)	−0.3534 (1)	0.0436 (4)
O2	0.2388 (1)	−0.0199 (1)	−0.3441 (1)	0.0460 (4)
C1	0.6516 (2)	0.0938 (1)	0.0093 (2)	0.0353 (5)
C2	0.5501 (2)	0.0440 (1)	−0.1777 (2)	0.0391 (5)
C3	0.3909 (2)	−0.0535 (1)	−0.2140 (2)	0.0372 (5)
C4	0.8025 (2)	0.1888 (1)	0.0145 (2)	0.0402 (5)
C5	0.9131 (2)	0.2502 (1)	0.1855 (2)	0.0426 (5)
C6	1.0584 (2)	0.3485 (1)	0.1857 (2)	0.0405 (5)
C7	1.1205 (2)	0.3768 (1)	0.0048 (2)	0.0487 (6)
C8	1.2530 (2)	0.4731 (2)	0.0142 (3)	0.0573 (7)
C9	1.3258 (2)	0.5432 (1)	0.2035 (3)	0.0611 (7)
C10	1.2673 (2)	0.5166 (2)	0.3843 (3)	0.0634 (8)
C11	1.1361 (2)	0.4194 (1)	0.3758 (2)	0.0526 (6)
C12	0.5679 (2)	−0.2039 (1)	−0.2794 (3)	0.0641 (7)
C13	0.1666 (2)	0.0734 (2)	−0.2545 (3)	0.0692 (8)
(II)				
Cl	0.0727 (1)	0.1876 (1)	0.6947 (1)	0.0821 (4)
O1	−0.5052 (1)	0.4140 (1)	−0.2780 (1)	0.0495 (7)
O2	−0.6274 (1)	0.3338 (1)	−0.1512 (2)	0.0490 (7)
C1	−0.4200 (2)	0.4393 (2)	0.1022 (2)	0.0362 (9)
C2	−0.4605 (2)	0.3756 (2)	−0.0181 (2)	0.0402 (9)
C3	−0.5425 (2)	0.4235 (2)	−0.1340 (2)	0.0392 (9)
C4	−0.3390 (2)	0.3769 (2)	0.2037 (2)	0.0406 (10)
C5	−0.2871 (2)	0.4285 (2)	0.3226 (2)	0.0428 (10)
C6	−0.2034 (2)	0.3641 (2)	0.4177 (2)	0.0405 (10)
C7	−0.1800 (2)	0.2323 (2)	0.4086 (3)	0.0524 (12)
C8	−0.0971 (2)	0.1773 (2)	0.4948 (3)	0.0580 (12)
C9	−0.0357 (2)	0.2541 (2)	0.5912 (2)	0.0511 (11)
C10	−0.0575 (2)	0.3830 (2)	0.6061 (3)	0.0600 (13)
C11	−0.1418 (2)	0.4369 (2)	0.5211 (2)	0.0559 (12)
C12	−0.4242 (2)	0.5021 (3)	−0.3089 (3)	0.0608 (13)
C13	−0.6876 (2)	0.3191 (3)	−0.0271 (3)	0.0689 (14)
(III)				
O1	0.0120 (2)	−0.2094 (2)	1.0715 (2)	0.074 (1)
O2	0.1189 (2)	−0.0920 (2)	1.2647 (2)	0.068 (1)
C1	0.0795 (2)	0.0367 (2)	0.9226 (3)	0.052 (1)
C2	0.1165 (2)	−0.0472 (3)	1.0209 (3)	0.059 (1)
C3	0.0440 (2)	−0.0946 (2)	1.1077 (3)	0.056 (1)
C4	0.1530 (2)	0.0823 (3)	0.8381 (3)	0.059 (1)
C5	0.2536 (2)	0.0379 (3)	0.8305 (3)	0.060 (1)
C6	0.3325 (2)	0.0831 (2)	0.7524 (3)	0.052 (1)
C7	0.3049 (2)	0.1814 (2)	0.6680 (3)	0.060 (1)
C8	0.3829 (2)	0.2204 (2)	0.5995 (3)	0.059 (1)
C9	0.4901 (2)	0.1632 (2)	0.6105 (3)	0.052 (1)
C10	0.5168 (2)	0.0658 (3)	0.6939 (3)	0.066 (1)
C11	0.4395 (2)	0.0260 (3)	0.7636 (3)	0.066 (1)
C12	0.1097 (3)	−0.2854 (3)	1.0896 (4)	0.102 (2)
C13	0.1500 (3)	0.0178 (3)	1.3261 (4)	0.084 (2)
C14	0.5738 (3)	0.2063 (3)	0.5322 (3)	0.075 (2)

Table 2. *Selected bond lengths* (Å)

	(I)	(II)	(III)
C1—C2	1.336 (2)	1.336 (3)	1.326 (4)
C1—C3′	1.517 (2)	1.528 (3)	1.507 (4)
C2—C3	1.503 (2)	1.501 (3)	1.495 (5)
C1—C4	1.468 (2)	1.472 (3)	1.479 (4)
C4—C5	1.331 (2)	1.325 (3)	1.300 (4)
C5—C6	1.471 (2)	1.472 (3)	1.480 (4)
O1—C3	1.427 (2)	1.420 (2)	1.419 (4)
O2—C3	1.423 (2)	1.422 (2)	1.426 (3)
O1—C12	1.411 (2)	1.419 (3)	1.402 (4)
O2—C13	1.408 (2)	1.413 (3)	1.418 (4)

The structure solutions of (I)–(III) were carried out with *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and refinements were performed by full-matrix least-squares techniques. The positions of the H atoms were calculated and refined isotropically. All calculations were performed with the *MolEN* package (Fair, 1990). The figures were plotted using *ORTEP* (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71839 (64 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SE1044]

References

Fair, C. K. (1990). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis*. Enraf–Nonius, Delft, The Netherlands.

Irngartinger, H., Lichtenthäler, J., Fenske, D. & Baum, G. (1993). *Z. Naturforsch. Teil B*, **48**, 1411–1418.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Liebich, B. W., Yvon, K. & Margaretha, P. (1976). *Acta Cryst.* B**32**, 269–271.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

Nørskov-Lauritsen, L. N., Larsen, S., Ettlinger, M. G. & Jaroszewski, J. W. (1982). *Acta Cryst.* B**38**, 3107–3110.

Acta Cryst. (1994). C**50**, 1156–1159

A Spiro-Indole Derivative, $C_{16}H_{10}ClFN_2O_2S$

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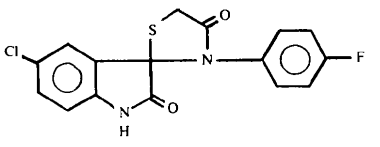
Abstract

The spiro-indole derivative, 5-chloro-3′-(4-fluorophenyl)spiro[3*H*-indole-3,2′-thiazolidine]-2,4′(1*H*)-dione, has been synthesized by the reaction of mer-

captoacetic acid with 5-chloroimino-3-(4-fluorophenyl)-2*H*-indol-2-one. The latter compound is prepared *in situ* from 5-chloroindole-2,3-dione and 4-fluoroaniline. The structure of the title compound confirms the conclusions drawn from the spectroscopic studies that the environment of the spiro C atom is based on tetrahedral geometry having bond angles in the range 109.6 (3)–117.3 (2)°.

Comment

In continuation of our earlier work on the synthesis of biologically active 3-phenylspiro[3*H*-indole-3,2′-thiazolidine)-2,4′-diones and related spiro-indole derivatives (Dandia, Kaur & Singh, 1992; Dandia, Khanna & Joshi, 1991; Joshi, Dandia & Sanan, 1989*a*,*b*; Joshi, Dandia & Ahmed, 1986, 1989), we have now investigated the crystal structure of one of the spiro derivatives. These spiro-indole derivatives exhibit antibacterial and antifungal properties (Danda, Kaur & Singh, 1993; Joshi, Dandia & Bhagat, 1990). A survey of the literature reveals that the structural features of spiro[indole-thiazolidine]-diones have not been studied so far. We have been able to obtain suitable crystals of only one synthesized thiazolidine derivative, $C_{16}H_{10}ClFN_2O_2S$ (I), and its structure is reported here. The molecular structure is shown in Fig. 1.



(I)

The C—F bond length of 1.374 (5) Å is similar to the value of 1.38 (2) Å reported for the 2-(4-fluorophenyl)benzoxazole dimer, $C_{26}H_{16}N_2O_2F_2$ (Paillous, Forgues, Jaud & Devillers, 1987). The C—N bonds C(4)—N(1) [1.399 (4) Å] and C(11)—N(2) [1.434 (5) Å] have a mean length of 1.416 (4) Å, which is very close to the reported value of 1.423 (15) Å for the 2-(4-fluorophenyl)bensoxazole dimer $C_{26}H_{16}N_2O_2F_2$ (Paillous, Forgues, Jaud & Devillers, 1987). The slightly longer C(8)—N(2) bond distance [1.451 (4) Å] of the title compound is probably a result of the spiro nature of the C(8) atom. The C(7)—N(1) and C(10)—N(2) bond distances are 1.347 (5) and 1.363 (4) Å, respectively, with a mean value of 1.355 (4) Å. The mean value is very close to the previously reported value of 1.364 (3) Å in pyrrolobenzazacyclododecine, $C_{20}H_{21}NO_4$ (Letcher, Lai & Mak, 1985). The slight shortening of the average distance of C(7)—N(1) and C(10)—N(2) [1.355 (4) Å] compared to the average distance of C(4)—N(1) and C(11)—N(2) [1.416 (4) Å] could result from the attachment of the highly electronegative carbonyl O atoms to the atoms C(7) and C(10).

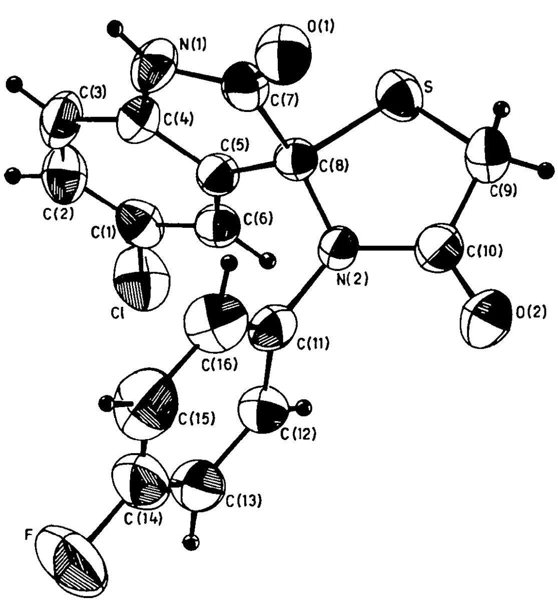


Fig. 1. Structure of $C_{16}H_{10}ClFN_2O_2S$.

The average value of the C=O bond lengths in the present compound [1.211 (4) Å] is equal to the C=O bond length [1.211 (3) Å] observed in pyrrolobenzazacyclododecine, $C_{20}H_{21}NO_4$ (Letcher, Lai & Mak, 1985). The average C—S bond length of 1.806 (3) Å is in good agreement with the corresponding C—S value [1.813 (4) Å] observed for dioxathiadiazaheteropentalene, $C_5H_4N_2O_2S_2$ (Camilleri, Rzepa, Slawin & Williams, 1989). The average value of the C—C bond distances in the fused phenyl ring of indole is 1.376 (4) Å, while in the isolated phenyl ring the corresponding value is 1.371 (5) Å. The environment of the spiro atom C(8) is nearly tetrahedral, having bond angles S—C(8)—C(7) = 109.6 (3), S—C(8)—C(5) = 111.3 (3), N(2)—C(8)—C(7) = 111.5 (2) and N(2)—C(8)—C(5) = 117.3 (2)°. The average value of the phenyl ring C—C—C bond angles is 120°.

On the basis of the spectroscopic data from ^{1}H and ^{13}C NMR measurements (Joshi, Dandia & Bhagat, 1990; Dandia, Kaur & Singh, 1993) the spiran system has been identified as 5-chloro-3′-(4-fluorophenyl)spiro[3*H*-indole-3,2′-thiazolidine]-2,4′(1*H*)-dione. The tentative structure proposed from these studies is in good agreement with the structure determined from the X-ray diffraction data.

Experimental

5-Chloro-3′-(4-fluorophenyl)spiro[3*H*-indole-3,2′-thiazolidine]-2,4′(1*H*)-dione is prepared by a one-step process. A mixture of 5-chloroindole-2,3-dione (1.81 g, 0.01 mol) and 4-

fluoroaniline (1.11 g, 0.01 mol) was refluxed in dry toulene for 2-3 h using Dean-Stark apparatus for azeotropical removal of water formed. After cooling the mixture, mercaptoacetic acid (1.38 g, 0.015 mol) was added and the reaction mixture refluxed again for 3-4 h under identical conditions. The whole mixture was then brought to room temperature and the excess solvent was removed under reduced pressure. The solid compound thus obtained was recrytallized from ethanol. Analysis: calculated for $C_{16}H_{10}ClFN_2O_2S$, C 55.17, H 2.87, N 8.04, S 9.19%; found, C 55.10, H 2.80, N 8.09, S 9.26%.

Crystal data

$C_{16}H_{10}ClFN_2O_2S$
$M_r = 348.79$
Monoclinic
$P2_1/c$
$a = 12.252$ (1) Å
$b = 8.158$ (3) Å
$c = 15.388$ (2) Å
$\beta = 95.79$ (8)°
$V = 1530.2$ Å^3
$Z = 4$

$D_x = 1.514$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 5$-12°
$\mu = 0.398$ mm^{-1}
$T = 295$ K
Plates
0.30 × 0.15 × 0.08 mm
Colourless

Data collection

Enraf-Nonius diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3100 measured reflections
2913 independent reflections
1627 observed reflections $[I > 3\sigma(I)]$

$R_{int} = 0.081$
$\theta_{max} = 25°$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 9$
$l = -18 \rightarrow 18$
2 standard reflections
frequency: 30 min
intensity variation: none

Refinement

Refinement on F
$R = 0.042$
$wR = 0.045$
1627 reflections
248 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F)$

$(\Delta/\sigma)_{max} = 0.06$
$\Delta\rho_{max} = 0.213$ e Å^{-3}
$\Delta\rho_{min} = 0.151$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *SDP-Plus* (Frenz, 1985)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
Cl	1.10254 (7)	0.2362 (1)	0.57025 (8)	6.37 (3)
S	0.65200 (7)	−0.0173 (1)	0.49155 (6)	3.70 (2)
F	0.8638 (3)	0.6476 (3)	0.1675 (2)	8.95 (7)
O(1)	0.4959 (2)	0.3027 (3)	0.4375 (2)	4.21 (5)
O(2)	0.6215 (2)	−0.0037 (3)	0.2414 (2)	6.42 (7)
N(1)	0.6393 (2)	0.4193 (3)	0.5244 (2)	3.88 (6)
N(2)	0.6843 (2)	0.1596 (3)	0.3552 (2)	3.07 (5)
C(1)	0.9662 (3)	0.2997 (5)	0.5564 (2)	4.10 (8)
C(2)	0.9359 (3)	0.4382 (5)	0.5987 (2)	4.79 (9)
C(3)	0.8276 (3)	0.4867 (4)	0.5922 (2)	4.74 (9)
C(4)	0.7524 (3)	0.3945 (4)	0.5414 (2)	3.42 (7)
C(5)	0.7831 (2)	0.2573 (4)	0.4975 (2)	3.01 (6)
C(6)	0.8908 (2)	0.2075 (4)	0.5045 (2)	3.45 (7)
C(7)	0.5913 (3)	0.3081 (4)	0.4683 (2)	3.38 (7)
C(8)	0.6825 (2)	0.1842 (4)	0.4484 (2)	2.91 (6)
C(9)	0.5902 (3)	−0.0841 (5)	0.3873 (2)	4.62 (8)
C(10)	0.6324 (3)	0.0247 (4)	0.3187 (2)	4.06 (8)
C(11)	0.7275 (3)	0.2862 (4)	0.3038 (2)	3.32 (7)
C(12)	0.8316 (3)	0.2690 (4)	0.2785 (2)	3.99 (8)
C(13)	0.8771 (3)	0.3903 (5)	0.2312 (2)	4.95 (9)
C(14)	0.8165 (4)	0.5249 (5)	0.2120 (2)	5.6 (1)
C(15)	0.7128 (4)	0.5476 (5)	0.2334 (3)	6.0 (1)
C(16)	0.6666 (3)	0.4244 (5)	0.2803 (2)	4.64 (8)

Table 2. *Selected geometric parameters* (Å, °)

Cl—C(1)	1.741 (3)	N(1)—C(7)	1.347 (5)
S—C(8)	1.825 (3)	N(2)—C(8)	1.451 (4)
S—C(9)	1.788 (4)	N(2)—C(10)	1.363 (4)
F—C(14)	1.374 (5)	N(2)—C(11)	1.434 (5)
O(1)—C(7)	1.217 (4)	C(5)—C(8)	1.504 (4)
O(2)—C(10)	1.206 (4)	C(7)—C(8)	1.561 (4)
N(1)—C(4)	1.399 (4)	C(9)—C(10)	1.510 (6)
C(8)—S—C(9)	91.8 (2)	C(5)—C(8)—C(7)	102.2 (2)
C(4)—N(1)—C(7)	112.5 (3)	S—C(9)—C(10)	107.8 (2)
C(8)—N(2)—C(10)	117.8 (3)	O(2)—C(10)—N(2)	124.2 (3)
C(8)—N(2)—C(11)	119.2 (2)	O(2)—C(10)—C(9)	124.5 (3)
C(10)—N(2)—C(11)	122.6 (3)	N(2)—C(10)—C(9)	111.4 (3)
Cl—C(1)—C(2)	119.3 (3)	N(2)—C(11)—C(12)	119.1 (3)
Cl—C(1)—C(6)	119.1 (3)	N(2)—C(11)—C(16)	120.9 (3)
N(1)—C(4)—C(3)	128.6 (4)	C(4)—C(5)—C(8)	108.5 (3)
N(1)—C(4)—C(5)	109.9 (3)	C(6)—C(5)—C(8)	130.9 (3)
S—C(8)—N(2)	105.0 (2)	O(1)—C(7)—N(1)	127.9 (3)
S—C(8)—C(5)	111.3 (3)	O(1)—C(7)—C(8)	125.4 (3)
S—C(8)—C(7)	109.6 (3)	N(1)—C(7)—C(8)	106.7 (2)
N(2)—C(8)—C(5)	117.3 (2)	F—C(14)—C(13)	117.0 (4)
N(2)—C(8)—C(7)	111.5 (2)	F—C(14)—C(15)	118.3 (4)

All calculations and computation were carried out on a PDP 11/73 computer, using *SDP-Plus* (Frenz, 1985).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71826 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1096]

References

Comilleri, P., Rzepa, H. S., Slawin, A. M. Z. & Williams, D. J. (1989). *J. Chem. Soc. Perkin Trans.* 2, pp. 469–474.

Dandia, A., Kaur, V. & Sing. P. (1992). *Phosphorus Sulfur Silicon*, **69**, 277-281.

Dandia, A., Kaur, V. & Singh, P. (1993). *Indian J. Pharm. Sci.* **55**, 129–136.

Dandia, A., Khanna, S. & Joshi, K. C. (1991). *Indian J. Chem.* **B30**, 469–472.

Frenz, B. A. (1985). *Enraf–Nonius SDP-Plus Structure Determination Package*. Version 3.0. Enraf–Nonius, Delft, The Netherlands.

Joshi, K. C., Dandia, A. & Sanan, S. (1989*a*). *J. Fluorine Chem.* **44**, 59–72.

Joshi, K. C., Dandia, A. & Sanan, S. (1989*b*). *J. Heterocycl. Chem.* **26**, 1397–1400.

Joshi, K. C., Dandia, A. & Ahmed, N. (1986). *Heterocycles*, **24**, 2479–2485.

Joshi, K. C., Dandia, A. & Ahmed, N. (1989). *Indian J. Chem.* **B28**, 639–641.

Joshi, K. C., Dandia, A. & Bhagat, S. (1990). *Indian J. Chem.* **B29**, 766–770.

Letcher, R. M., Lai, T. F. & Mak, T. C. W. (1985). *J. Chem. Soc. Perkin Trans.* 1, pp. 1921–1926.

Paillous, N., Forgues, S. F., Jaud, J. & Devillers, J. (1987). *J. Chem. Soc. Chem. Commun.* pp. 578–579.

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1-Acetyl-5-benzyl-2-methylthio-5*H*-imidazol-4-one

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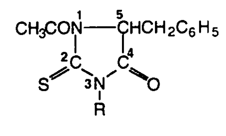
Abstract

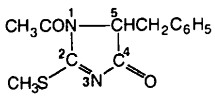
Atoms of the imidazolone ring in the title compound, $C_{13}H_{14}N_2O_2S$, are approximately coplanar. The N(1) acetyl group lies close to the plane while the C(2) methylthio substituent is twisted by about 7° from it. The imidazolone and phenyl rings face each other, the dihedral angle between their perpendiculars being 53.4 (3)°.

Comment

The methylation of 1-acetyl-5-benzyl-2-thioxoimidazolidin-4-one [*N*-acetylphenylalanine thiohydantoin (1), *R* = H] by means of diazomethane has been studied, and the reaction, experimental details of which will be reported elsewhere, found to give two isomers, namely the *N*-methyl isomer [(1), $R = CH_3$] and the *S*-methyl isomer (2). The structure of the former isomer was established by means of its ^{1}H NMR spectrum (the relevant spectroscopic data will be presented elsewhere) as 1-acetyl-5-benzyl-3-methyl-2-thioxoimidazolidin-4-one [(1), $R = CH_3$]. The structure of the latter isomer was shown by X-ray analysis to be 1-acetyl-5-benzyl-2-methylthio-5*H*-imidazol-4-one (2).



(1)



(2)

The atoms of the imidazolone ring are coplanar to within 0.038 (5) Å, but there is a slight degree of ring pucker, as reflected in the ring torsion angles (Table 2); the acetyl group at N(1) lies close to the ring plane [torsion angle C(5)—N(1)—C(1′)—C(1″) 2.6 (4)°], while the S—CH_3 group at C(2) is twisted by about 7° from it. The benzyl group at C(5) adopts an orientation relative to the imidazolone moiety as defined by the torsion angles C(4)—C(5)—C(5′)—C(6′) of 57.1 (3)° and C(5)—C(5′)—C(6′)—C(7′) of 81.9 (3)°. The two rings face each other, the dihedral angle between their perpendiculars being 53.4 (3)° (see Fig. 2). When compared with other 2-thiohydantoin derivatives (Lempert, Nyitrai, Zauer, Kálmán, Argay, Duisenberg & Sohar, 1973; Kiéc-Kononowicz, Zejc, Mikolajczyk, Zatorski, Karolak-

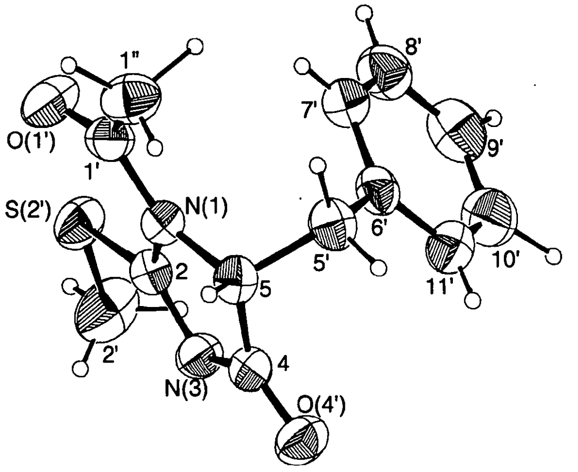


Fig. 1. Perspective view of (2) (3*R* enantiomer) with displacement ellipsoids scaled to 50% probability. The C symbol for C atoms is omitted and H atoms are denoted by spheres of arbitrary radii.

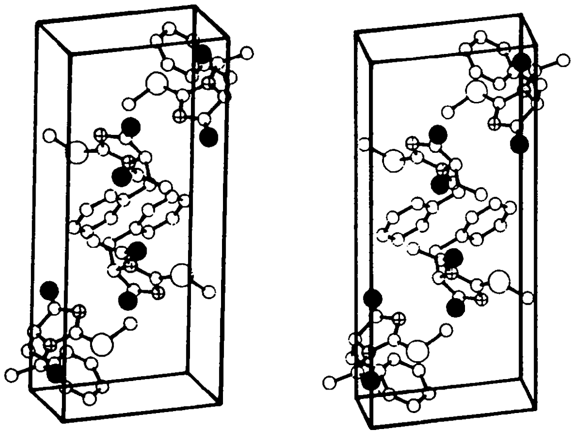


Fig. 2. Stereoview of the crystal packing, projected along **a** with the *b* axis vertical.

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