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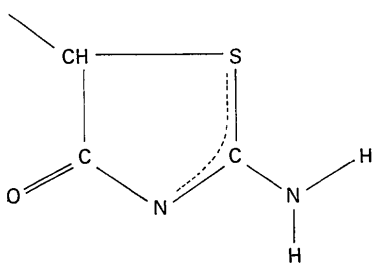

Fig. 4. Structure of the heterocyclic ring showing the partial conjugation.

Table 3. *Intermolecular contact distances shorter than 3·5 Å with e.s.d.'s in parentheses*

First designated atom of each pair belongs to the reference molecule and has the coordinates x,y,z listed in Table 1.

		Symmetry operation applied to 2nd atom
C(1)–N(1)	3·340 (9)	*A*
C(4)–O(2)	3·468 (9)	*B*
C(5)–O(3)	3·404 (14)	*C*
*N(1)–O(2)	2·598 (9)	*B*
*N(2)–O(1)	2·881 (9)	*B*
*N(2)–O(3)	2·841 (10)	*C*

Key to symmetry operations

A $1-x, \frac{1}{2}-y, \frac{1}{2}-z$
B $1+x, \frac{1}{2}-y, \frac{1}{2}+z$
C $x, \frac{1}{2}-y, \frac{1}{2}+z$

* Hydrogen bonds

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The Crystal and Molecular Structure of Sulphur-Containing Heterocyclic Ring Compounds. II. 2-Imino-4-thiazolidinone

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2-Imino-4-thiazolidinone, $C_3H_4N_2OS$, is monoclinic, space group $P2_1/n$, $Z=4$. The structure was solved by Patterson and minimum function methods with 467 visually estimated reflexions, and refined to $R=0{\cdot}115$. The molecule is planar. The bond lengths and the proposed hydrogen bonding in the crystal suggest that the heterocyclic ring exists almost as 2-imino with much less conjugation than the ring in 2-amino-4-thiazolidinone-5-acetic. acid.

Introduction

The structure analysis of 2-imino-4-thiazolidinone, $C_3H_4N_2OS$, has been undertaken to determine the amount of conjugation of the 5-membered ring compared with that in 2-amino-4-thiazolidinone-5-acetic acid (Amirthalingam & Muralidharan, 1972, hereafter referred to as A & M), and to discover whether the compound exists in the 2-amino or the 2-imino form.

Experimental

The crystals were colourless, monoclinic needles. The unit-cell parameters derived from Weissenberg photographs with Cu $K\alpha$ radiation ($\lambda=1{\cdot}542$ Å) are:

$a=4{\cdot}09$ (1), $b=9{\cdot}05$ (1), $c=13{\cdot}15$ (2) Å, $\beta=93{\cdot}0$ (5)°
$Z=4$, $d_o=1{\cdot}56$ g.cm^{-3}, $d_c=1{\cdot}59$ g.cm^{-3}.

The systematic absences $h0l$ with $h+l$ odd and $0k0$ with k odd characterize the space group uniquely as $P2_1/n$.

The reflexions nkl ($n=0$ to 2) and $h0l$ were recorded by the equi-inclination Weissenberg technique with Cu $K\alpha$ radiation and their intensities measured visually. The 467 unique reflexions were corrected for Lorentz and polarization effects and for spot size, but not for absorption. Initially the scaling of the nkl reflexions was done by Wilson plots.

The $0kl$ projection was solved by Patterson and minimum function methods, yielding positions of all the non-hydrogen atoms, and refined to $R=0{\cdot}12$. The x coordinates were assigned from packing considerations and the structure refined with anisotropic temperature factors for the sulphur atom only. Form factors were taken from *International Tables for X-ray Crystallography* (1962). Hydrogen atoms were ignored. In the final stages of the full-matrix least-squares refinement Cruickshank's weighting scheme $\sigma=(5{\cdot}0+F_o+0{\cdot}03F_o^2)$ was used. The final R for all observed reflexions was 0·115.

Table 1. *Final positional and thermal parameters of the atoms with esd's in parentheses*

	x	y	z	B
S	0·8090 (11)	0·1118 (2)	0·0890 (2)	–
O	0·3765 (31)	0·3623 (8)	0·2776 (6)	3·0 (2)
C(1)	0·6616 (41)	0·1485 (12)	0·2102 (8)	2·8 (2)
C(2)	0·5015 (37)	0·3042 (9)	0·2038 (7)	2·2 (2)
C(3)	0·6774 (37)	0·2888 (10)	0·0449 (8)	2·5 (2)
N(1)	0·5329 (35)	0·3739 (8)	0·1124 (7)	2·5 (2)
N(2)	0·7245 (34)	0·3282 (10)	−0·0487 (7)	3·1 (2)

Anisotropic temperature factor for sulphur of the form

$\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{23}kl+2\beta_{13}hl)]$

β_{11}	β_{22}	β_{33}
0·2848 (57)	0·0080 (3)	0·0037 (1)
β_{12}	β_{23}	β_{13}
0·0087 (13)	−0·0005 (2)	0·0056 (15)

Description of the structure

The structure projected down **a** is shown in Fig. 1 with possible hydrogen bonds included. The final parameters are given in Table 1. Table 2 lists F_o and F_c for all observed reflexions. Bond lengths and angles are shown in Fig. 2.

The molecule is planar (Table 3). The bond lengths (Fig. 2) show that C(3)–N(2) is almost a double bond and that there is less conjugation in the ring compared with that in 2-amino-4-thiazolidinone-5-acetic (A & M). Furthermore the hydrogen bonds (Fig. 1) in the crystal, which are of the types N–H···O (2·95 Å) and N–H...N (3·00 Å) show that the compound is in the 2-imino rather than in the 2-amino form.

An analysis of the intermolecular contacts (Table 4) shows that the S···O contact at 3·10 Å is rather short, but somewhat greater than the S···O intramolecular distance of 2·96 Å found in 2-amino-4-thiazolidinone-5-acetic acid. The C(1)–S···O angle is 77° whereas the corresponding angle obtained in the compound with the acetic acid side chain in the 5-position was 65° (A & M). Thus it is clear that the S···O interaction does play a part in dictating the state of conjugation in the ring and, since the S···O distance is

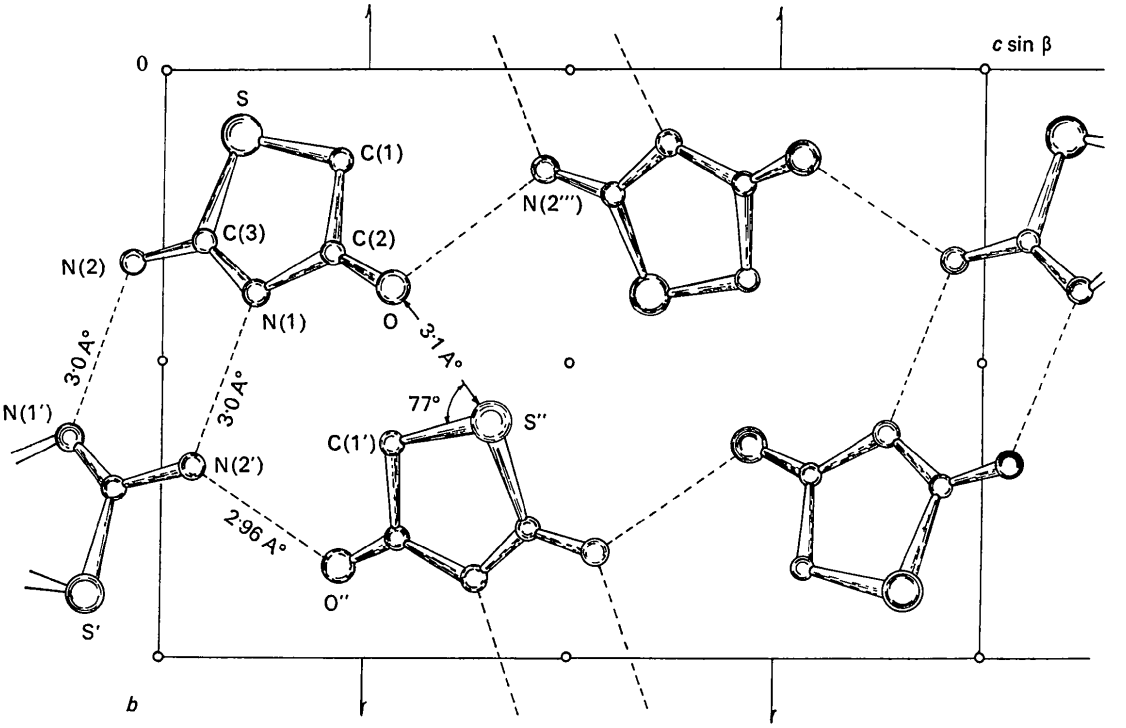
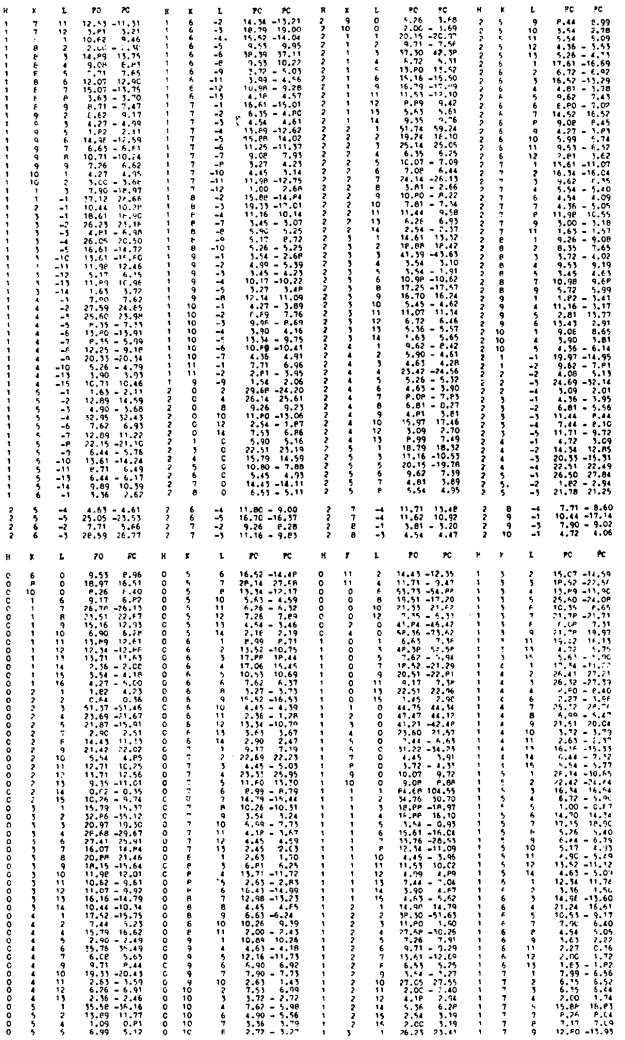


Fig. 1. The structure viewed in projection down **a**. Dotted lines shows possible hydrogen bonds. The S···O intermolecular contact is also shown.

Table 2. *Observed and calculated structure parameters*



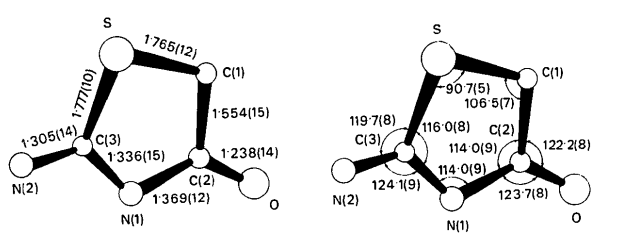


Fig. 2. Bond lengths and angles with e.s.d.'s in parentheses.

Table 3. *The equation of the mean plane of the molecule and deviations from this plane*

$0{\cdot}8671x+0{\cdot}3912y+0{\cdot}3081z=3{\cdot}5756$

S	0·007 Å
C(1)	0·014
C(2)	0·016
C(3)	0·003
N(1)	0·022
N(2)	0·009
O	0·008

Table 4. *Intermolecular distances shorter than* 3·5 Å *with esd's in parentheses*

First designated atom of each pair belongs to reference molecule and has the coordinates x, y, z, listed in Table 1.

		Symmetry operation applied to 2nd atom
S–O	3·096 (8)	*A*
O–C(1)	3·204 (16)	*B*
O–C(1)	3·407 (17)	*C*
*N(1)–N(2)	2·998 (13)	*D*
*O–N(2)	2·954 (13)	*E*

*Hydrogen bonds

Key to symmetry operation.

A	$1+(\frac{1}{2}-x),\ \frac{1}{2}-y,\ \frac{1}{2}-z$
B	$1+(\frac{1}{2}-x),\ \frac{1}{2}+y,\ \frac{1}{2}-z$
C	$\frac{1}{2}-x,\ \frac{1}{2}+y,\ \frac{1}{2}-z$
D	$1-x,\ 1-y,\ -z$
E	$\frac{1}{2}+x,\ \frac{1}{2}-y,\ \frac{1}{2}-z$

greater here, the conjugation becomes less (Johnson, Maier & Paul, 1970).

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