The Crystal and Molecular Structure of 2-Amino-4-thiazolidinone-5-acetic Acid

By V. AMIRTHALINGAM* and K. V. MURALIDHARAN

(*Chemistry Division, Bhabha Atomic Research Centre, Trombay, Bombay-85, India*)

Summary 2-Amino-4-thiazolidinone-5-acetic acid, a potential radioprotective agent, is found to be more 2-amino- than 2-imino-.

THE needle shaped crystals of 2-amino-4-thiazolidinone-5-acetic acid belong to the monoclinic system with space group $P2_1/c$. The unit-cell parameters are $a = 10{\cdot}30 \pm 0{\cdot}02$, $b = 7{\cdot}32 \pm 0{\cdot}01$, $c = 12{\cdot}64 \pm 0{\cdot}02$ Å; $\beta = 128° \pm 1°$, $Z = 4$.[1]

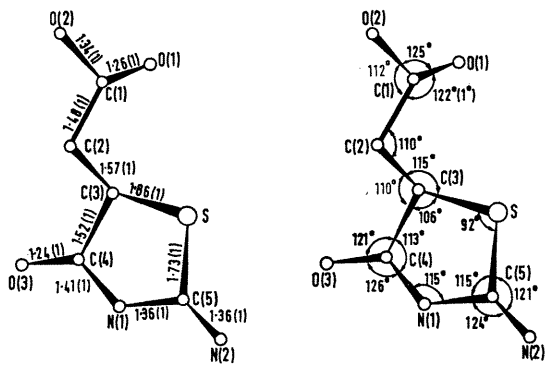


FIGURE 1. *The bond lengths and angles of the molecule. Values in parentheses are the e.s.ds.*

The X-ray intensity data for 957 reflections were obtained from equi-inclination Weissenberg photographs by visual estimation. The structure was deduced essentially by the heavy-atom method by locating the sulphur atom from three-dimensional Patterson synthesis. All the other atoms were located by successive Fourier methods. The parameters, with anisotropic temperature factors for sulphur, were refined by full-matrix least-squares to $R = 0{\cdot}11$.

The final bond angle and lengths of the molecule are given in Figure 1. The partial double bond character of S–C(5), N(1)–C(5), and N(2)–C(5) are clear. The carboxy-group is planar. The five-membered ring, together with O(3) and N(2) is nearly planar. Hydrogen bonding in the crystal (as shown in Figure 2) is of the types N–H · · · · · O and O–H · · · · · · N. These results indicate that the

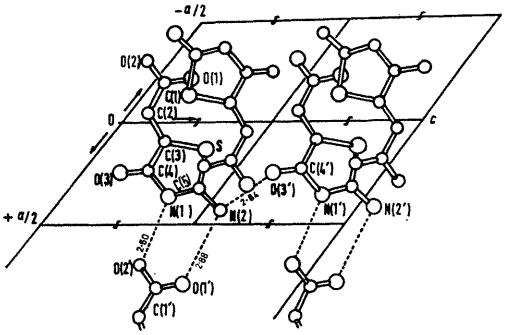
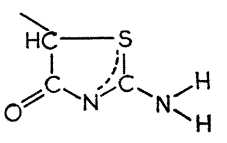


FIGURE 2. *Structure viewed down the* b*-axis, showing the possible hydrogen bonding by dotted lines.*

structure of the five-membered ring is (I) and the compound is more 2-amino- than 2-imino- in character.



(I)

(*Received, July 7th,* 1969; *Com.* 986.)

[1] V. Amirthalingam and K. V. Muralidharan, *Indian J. Pure Appl. Phys.*, 1967, **5**, 373.