The Crystal Structure of 2-Imino-5-phenyl-4-thiazolidinone

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Summary The zwitterionic structure of the five-membered ring in 2-imino-5-phenyl-4-thiazolidinone is clearly demonstrated for the first time.

THE crystal structure of 2-imino-5-phenyl-4-thiazolidinone was undertaken to help establish the zwitterionic structure of the five-membered ring.

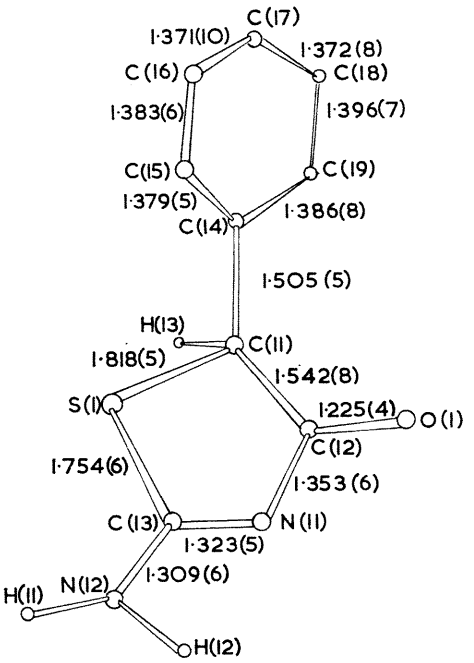
Clear plate-like crystals of $C_9H_8ON_2S$ were grown from ethanol.[1] *Crystal data*: $C_9H_8ON_2S$; M, 192.; Monoclinic; $a = 8{\cdot}591(1)$, $b = 33{\cdot}051(22)$, $c = 6{\cdot}713(3)$ Å, $\beta = 106{\cdot}54(1)°$; $U = 1827{\cdot}10$ Å^3; $D_m = 1{\cdot}398(1)$ (by flotation); $Z = 8$, $D_c = 1{\cdot}405$; $F(000) = 912$; space group $P2_1/c$, Mo-K_α radiation, niobium filtered, single crystal General Electric XRD6 automated diffractometer. 4128 independent measurements were made using the ω–2θ scan technique.

The co-ordinates for the sulphur, oxygen, carbon, and nitrogen (non-hydrogen) atoms were obtained from direct methods.[2] Two independent molecules were determined and a conventional R value of 0·18 was obtained from the initial positions interpreted from the E-map. Refinement using full-matrix least-squares brought the R value to 0·138 for individual isotropic temperature factors. The hydrogen atoms were located with the aid of a Fourier difference map. Anisotropic refinement on the non-hydrogen atoms and isotropic refinement on the hydrogen atoms brought the R value to 0·048.

The interatomic distances are shown in the Figure. Of particular interest is the observation that the distances of 1·323(5) Å between C(13) and N(11), 1·309(6) Å between C(13) and N(12), and 1·353(6) Å between C(12) and N(11) are significantly shorter than the 1·47(02) Å postulated by Pauling as a typical C–N single bond.[3] The location of two hydrogens on N(12) and the short C–N distances confirm the speculation that a zwitterionic form exists.

The hydrogen-bonding network forms chains of molecules along the short c-axis bonded O(1) to S(1) and O(1) to N(12) with distances of 3·26(1) and 2·78(1) Å, respectively.

We thank the Walter Reed Army Medical Center for the use of the G. E. XRD-6 automated diffractometer and NASA for support of the computing.



FIGURE

(*Received, May 30th,* 1969; *Com.* 760.)

[1] W. Reeve and M. Nees, *J. Amer. Chem. Soc.*, 1967, **89**, 647.
[2] "X-Ray 67-Program System for X-Ray Crystallography," Technical Report 67—58, Computer Science Centre, University of Maryland, Dec., 1967.
[3] L. Pauling, "The Nature of the Chemical Bond," 3rd edn., Cornell University Press, Ithaca, 1960.