The Crystal Structure of Ethyl 2-Imino-4-oxo-5-phenylimidazolidine-1-carboximidate

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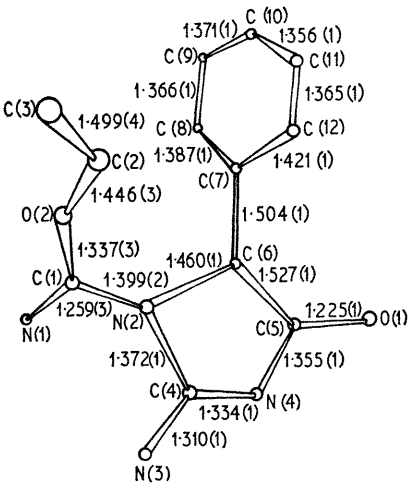
Summary The zwitterionic nature of the five-membered ring in ethyl 2-imino-4-oxo-5-phenylimidazolidine-1-carboximidate is shown for the first time.

THE crystal structure of ethyl 2-imino-4-oxo-5-phenylimidazolidine-1-carboximidate was undertaken to help establish the zwitterionic structure of the five-membered ring. The compound is also of interest on account of its antimalarial properties.

Clear plate-like crystals of $C_{12}H_{14}N_4O_2$ were grown from ethanol.[1] *Crystal data*: $C_{12}H_{14}N_4O_2$: M 246; monoclinic; $a = 11{\cdot}169(2)$ Å, $b = 11{\cdot}221(3)$, $c = 20{\cdot}453(13)$ Å; $\beta = 98{\cdot}12(1)°$; $U = 2537{\cdot}79$ Å^3; $D_m = 1{\cdot}280(5)$; $Z = 8$, $D_c = 1{\cdot}2875$; space group $P2_1/n$, 5698 independent intensity measurements were made using niobium-filtered Mo-K_α radiation, a single-crystal General Electric XRD-6 automated diffractometer and a combination of ω-2θ scans and stationary crystal-stationary counter techniques.

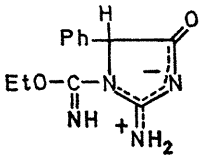
The co-ordinates for carbon, nitrogen, and oxygen (non-hydrogen) atoms were obtained from direct methods.[2] Two independent molecules were determined to give an R value of 0·124 for individual isotropic temperature factors. The hydrogen atoms were located with the aid of a Fourier difference map. Anisotropic refinement on the non-hydrogen atoms and positional refinement on the hydrogen atoms brought the R index to 0·048.

The interatomic distances are shown in the Figure. The five-membered imidazole ring is coplanar within 0·014 Å. Two hydrogen atoms were located on N(3) and one hydrogen atom was found joined to C(6). The length of N(2)–C(6) (1·46 Å) is typical of an N–C single bond (1·47 Å),[3] but the other three N–C bonds are significantly shorter. The C(4)–N(3) bond (1·31 Å) contains approximately 60%



FIGURE

double-bond character, and along with the other bond lengths indicates the following zwitterionic structure.



The phenyl group forms an 82° angle with the imidazole ring.

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