The Structure of Crystalline Cytidylic Acid b

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The crystal and molecular structure of cytidylic acid b is being investigated by X-ray diffraction methods. So far the main features of the structure have been established.

The crystal symmetry and the dimensions of the unit cell were derived from oscillation and Weissenberg photographs, taken with filtered copper radiation (λ = 1.542 Å). The crystals are orthorhombic, with space group $P2_12_12$, and unit cell dimensions [1]: a = 8.74 Å, b = 21.4 Å, c = 6.82 Å. The unit cell contains four molecules $C_9H_{14}N_3O_8P$. Weissenberg diagrams of the zones $hk0$-$hk4$ and $0kl$-$5kl$ were taken, and about 1 300 reflexes were recorded. The intensities were estimated visually.

Patterson projections along the two shortest axes indicated several possibilities for the position of the phosphorus atom. By the aid of three Harker sections and vector convergence maps [2] all of these except one were ruled out as improbable. The c-projection was very difficult to attack directly, as few unitary structure factors are larger than 0.15, and several attempts failed. It was then decided to try the a-projection, as the distribution of intensities in the $0kl$ zone seemed more favourable, though serious overlapping of atoms had to be expected.

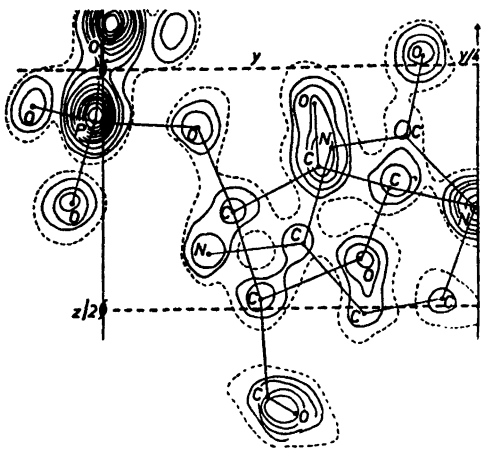

Fig. 1. Electron density projection along the a axis, showing one asymmetric unit. Plane group *pgm*. Contours at arbitrary but equal intervals.

It was found possible to derive the probable phases of four reflexes from an analysis of the distribution of vectors along the lines $x = 1/2$ and $z = 0$ in the two Patterson projections. From the distribution of positive and negative areas in the vector convergence map of the a-projection it could be concluded that the two largest structure factors should probably have opposite signs. One of these and one sign more could be chosen arbitrarily.

With these seven phases as a starting point a set of 22 probable phases was found by Harker-Kasper inequalities, using a high artificial temperature factor. The corresponding Fourier map was unclear, but indicated the positions of the oxygen atoms of the phosphate group. These were confirmed by the three-dimensional Patterson function. The rest of the molecule was then placed roughly by trial and error, and the structure refined by F_o and $(F_o - F_c)$ syntheses.

At the present stage the electron density map of the a-projection shows no false maxima, and the reliability index R is 0.30. We hope to be able to publish a full report on the work and a detailed discussion of the structure in the near future. So far it can only be said with a high degree of certainty that the phosphate group is bound to the ribose ring in the 3′ position, as should be expected [3].

We want to express our thanks to *Norges Almenvitenskapelige Forskningsråd*, whose financial support made this work possible.

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3. Fox, J. J., Cavalieri, L. F. and Chang, N. *J. Am. Chem. Soc.* **75** (1953) 4315.

Received December 15, 1956.