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The crystal structure of 5′-Br-3′:5′-dideoxythymidine.

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The X-ray analysis of 5′-Br-3′:5′-dideoxythymidine, which was produced during the study of the chemistry of certain thymidine derivatives (Michelson & Todd, 1955), was undertaken for the purpose of determining its chemical structure.

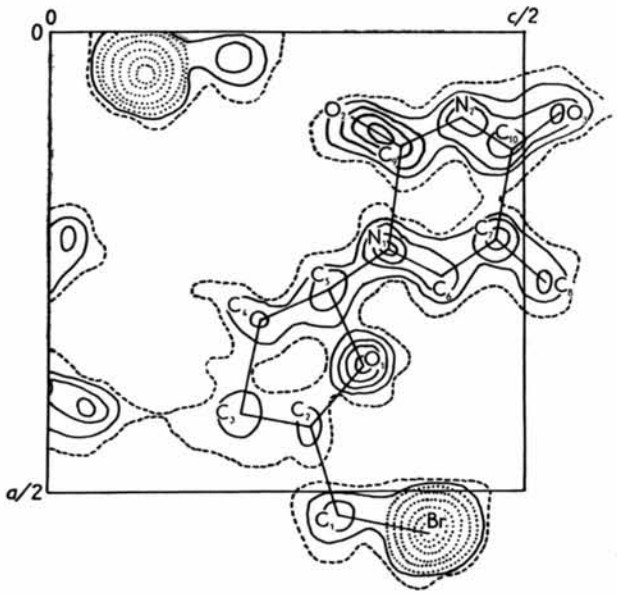

Fig. 1. 5′-Br-3′ : 5′-dideoxythymidine, electron-density map. The contours are at equal arbitrary intervals with the lowest contour broken. The dotted contours round the bromine atom are at twice the interval elsewhere.

The space group was found to be $P2_12_12_1$ with

$$a = 14{\cdot}78,\ b = 4{\cdot}89,\ c = 15{\cdot}17\ \text{Å},$$

there being four molecules per unit cell. The bromine parameters were readily found for the *h*0*l* projection from the two-dimensional Patterson synthesis. With the signs of the structure factors taken from the bromine contribution, an electron-density map was calculated which showed clearly the remainder of the atoms. One stage of refinement gave the map shown in Fig. 1, and, since the object of the investigation had been achieved, no further refinement was attempted. The atomic co-ordinates found for this projection are:

	x	*z*		*x*	*z*
C_1	0·533	0·304	O_1	0·364	0·330
C_2	0·430	0·274	O_2	0·091	0·318
C_3	0·416	0·202	O_3	0·089	0·535
C_4	0·314	0·221	N_1	0·236	0·356
C_5	0·280	0·294	N_2	0·093	0·434
C_6	0·266	0·413	Br	0·547	0·400
C_7	0·226	0·471			
C_8	0·274	0·522			
C_9	0·124	0·367			
C_{10}	0·128	0·486			

Reference

Michelson, A. M. & Todd, A. R. (1955). *J. Chem. Soc.* p. 816.

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The shrinkage of ribonuclease.

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In the course of taking an X-ray photograph to record the *h*0*l* reflexions of a wet ribonuclease crystal of the monoclinic form (ex aqueous alcohol) in a sealed capillary in the normal manner, a small leak allowed the crystal to dry during its exposure. There was recorded on the photograph both the diffraction pattern of the wet crystal and that of the dry one, with smear lines indicating that a change had taken place. This is most clearly seen (Fig. 1) for the 003 reflexion. The unit-cell dimensions of this form of ribonuclease are:

	a (Å)	*b* (Å)	*c* (Å)	*β* (°)
Wet	30·90	38·8	54·06	106
Dry	29·10	30·08	51·03	114·0

It was possible to confirm from this photograph that the angle *β* increases when the crystal goes from the wet to the dry state.

The crystal did not move off the capillary wall during the drying process and so Fig. 1 shows the correct orien-

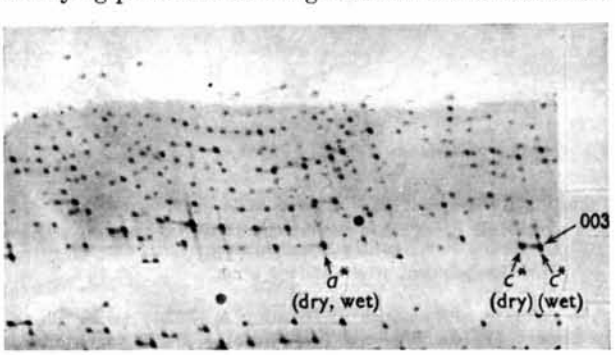

Fig. 1. Weissenberg photograph of ribonuclease, *h*0*l* reflexions.