CRYSTALLOGRAPHIC STUDIES ON LUTEOSKYRINE

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Received 10 December 1968

Luteoskyrin, a toxic pigment produced by Penicillum Islandicum [1] has been shown to bind to purine residues in single stranded nucleic acid in the presence of Mg^{++} ions [2]. The stoichiometry of this association is one pigment molecule and one Mg^{++} for one purine residue, with the restriction that a second purine residue, if vicinal, is not able to bind luteoskyrin probably as a result of steric hindrance. To elucidate the structure of the luteoskyrin-Mg-purine complex, the structure of luteoskyrin has to be known in great detail. Shibata and his group have greatly improved our knowledge in this field by NMR studies on rubroskyrin triacetate, derivative of a pigment closely related to luteoskyrin [3,4] and by X-ray diffraction studies on bromotetrahydrorugulosin [5]. In the meantime we have studied the crystal parameters of luteoskyrin itself. Monocrystals of luteoskyrin were obtained by addition of heptane to a saturated acetonic solution of the pure pigment [6].

The lattice constants of the orthorhombic unit cell were determined from oscillation and zero-level Weissenberg photographs about two crystallographic axes, a and c, with Cu $K\alpha_1$ (λ = 1.5405 Å) radiation.

Cell constants determined from rotation and Weissenberg photographs are as follows:

$a = 14.75 \pm 0.05$ Å
$b = 15.95 \pm 0.05$ Å
$c = 12.04 \pm 0.02$ Å

Equi-inclination Weissenberg photographs, $hk0 - hk6$, $0kl$, were taken on a Nonius camera, systematic abscissae of $h00$ for h odd, $0k0$ for k odd, indicate the space group to be $P_{2_12_12}$ [7].

The cell contains four formula units of $C_{30}H_{22}O_{12}$; the observed density is 1.38 g cm^{-3} (22°C), calculated 1.35 g cm^{-3}. This density has been observed by flottation by means of Mohr's scales with a solution of silver nitrate of which the pH was made close to one by addition of a few drops of nitric acid. The results of the density measurements show that the crystals had not grown and were not obtained in solvated form.

Two-dimensional Patterson analysis is now under progress to estimate the coordinates of atoms, the interatomic distances and the bond angles.

References

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