Tetrahedron Letters No.2, pp. 209-211, 1968. Pergamon Press Ltd. Printed in Great Britain.

THE CRYSTAL STRUCTURE OF PYRROLNITRIN

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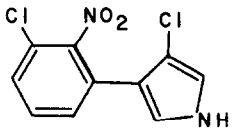
(Received in Japan 14 September 1967)

The chemical structure determination of pyrrolnitrin (I), an antibiotic isolated from a Pseudomonas, was reported by K.Arima, et al[1]. and the total synthesis was accomplished by H.Nakano, et al[2]. The X-ray analysis of the antibiotic is investigated, in order to determine its configuration and the intermolecular interactions in the crystalline state.



(I)

Single crystals were obtained on slow evaporation from the benzene solution. The crystal data were determined from the rotation and the Weisenberg photographs. The crystal belongs to the triclinic system (space group $P\bar{1}$) with a=7.91 A, b=11.58 A, c=7.58 A, $\alpha=97^{\circ}30'$, $\beta=119^{\circ}50'$, and $\gamma=110^{\circ}15'$. The observed density, 1.74 g/cm^3, indicated that the unit cell contains two molecules. Three dimentional diffraction intensities were visually estimated from the Weisenberg photographs about the b- and the c- axes with Cu Kα radiation.

The three dimentional Patterson function was calculated from 1899 independent data, and the minium function treatments revealed the location of

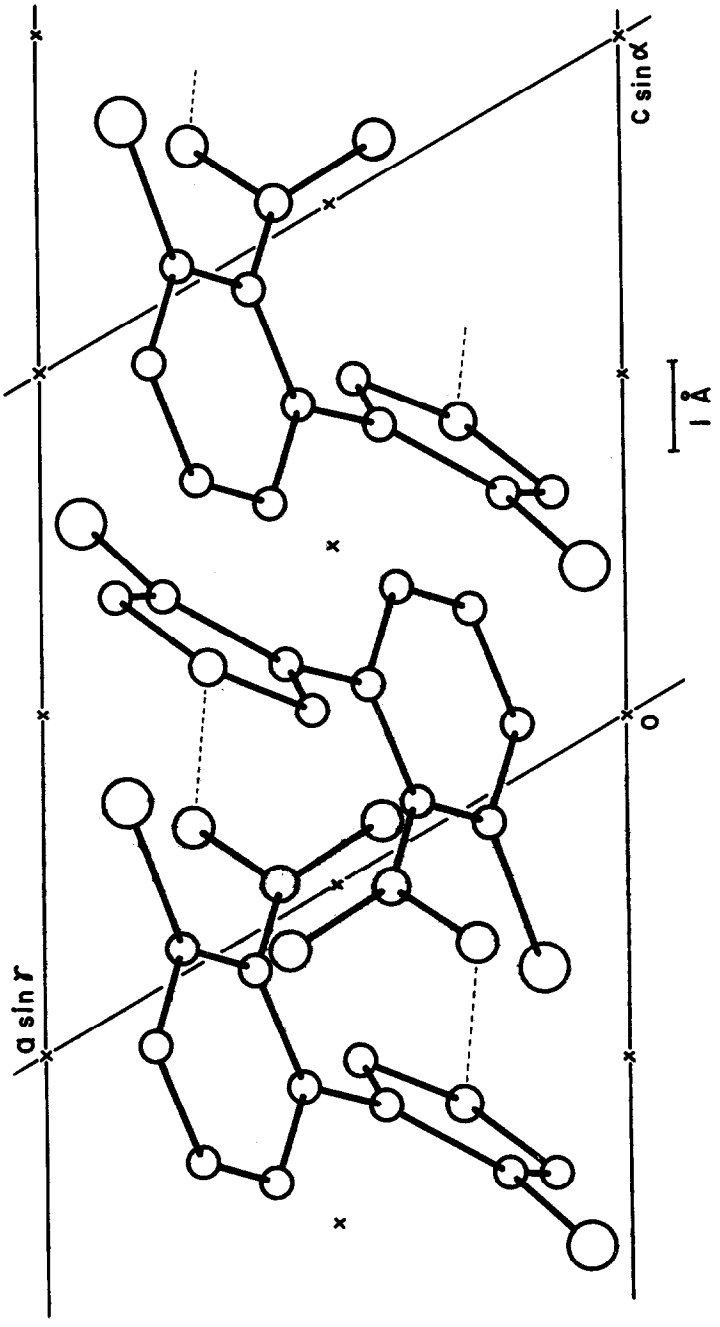


FIG. 1 The crystal structure of pyrrolnitrin

the two chlorine atoms in the asymmetrical unit. Successive applications of the usual Fourier syntheses and the least-square methods revealed the positions of the other atoms. The final R-factor, with anisotropic temperature factors for the chlorine atoms, is 0.140 for all independent reflections. The molecular arrangement in the unit cell projected along the b-axis is shown in Figure 1.

The dihedral angle of the pyrrole and the benzene rings is 52°, the chlorine substituent on the pyrrole ring being located apart from the nitro group. The plane through the nitro group is almost at right angle to the plane of the benzene ring (the angle; 88°).

In the unit cell, the two molecules lie opposite to each other about the center of symmetry as shown in Figure 1. One molecule seems to interact with the other molecule, through a weak intermolecular hydrogen bonding between the NH group of the pyrrole ring and the oxygen atom of the nitro group, to make up a dimer structure (interatomic distance; 3.060 0.008 A).

Full details will be published later.

The authors are grateful to Dr. K.Nakatsu, Osaka Municipal University and Dr. N.Sakabe, Nagoya University for their help in this work.

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