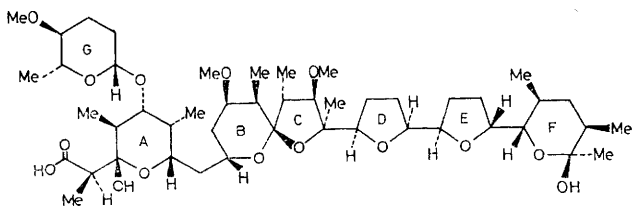
X-Ray Crystal Structure of the Thallium Salt of Carriomycin, a New Polyether Antibiotic

By NOBORU ŌTAKE,* HIROSHI NAKAYAMA, HIROSHI MIYAMAE,† SHOICHI SATO,† and YOSHIHIKO SAITO†

(*Institute of Applied Microbiology and* †*Institute for Solid State Physics, University of Tokyo, Tokyo* 113, *Japan*)

Summary The molecular structure of the antibiotic carriomycin has been established by *X*-ray crystallographic analysis of the thallium salt, $C_{47}H_{79}O_{15}Tl$.

CARRIOMYCIN[1] is a new antibiotic from *Streptomyces hygroscopicus* which shows antimicrobial activity against gram-positive bacteria, mycobacteria, yeast, and fungi and is an effective anticoccidial agent. Based on its physicochemical properties and its biological activity, carriomycin is believed to belong to the family of polyether antibiotics including monensin,[2] nigericin,[3] lasalocid A,[4] A-204A,[5] septamycin,[6] dianemycin,[7] Ro 21-6150,[8] salinomycin,[9] lysocellin,[10] and lonomycin.[11] It was isolated from a culture of the producing organism as a free monocarboxylic acid as crystalline needles, m.p. 120—122 °C, or as the sodium salt, m.p. 180—182 °C, $[\alpha]_D^{25}$ −4·5 (*c* 1, $CHCl_3$), ν_{max} (KBr) 1605 cm^{-1} (CO_2^-). The n.m.r. spectrum ($CDCl_3$) of the



(I)

latter shows the presence of three methoxy singlets in the region δ4·50—4·68. The molecular formula $C_{47}H_{79}NaO_{15}$ was confirmed by elemental analysis and the structure of carriomycin has been established as (I) by a three-dimensional *X*-ray analysis of the thallium salt.

Crystal data: $C_{47}H_{79}O_{15}Tl$, space group $P2_1$, a = 15·416, b = 12·325, c = 14·442 Å, β = 105·42°, D_m = 1·37 (flota-

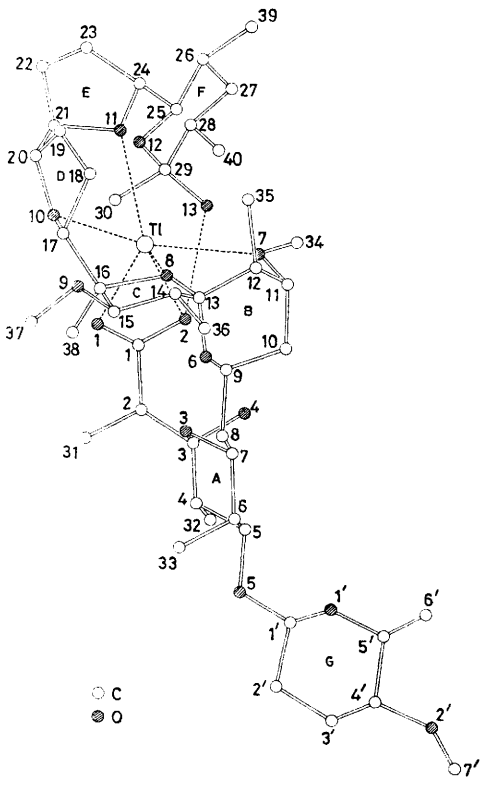


FIGURE. The molecular structure of the thallium salt of carriomycin viewed along *b* axis.

tion in aqueous KI), $D_c = 1{\cdot}38$ g cm^{-3}, $Z = 2$. The intensity data were collected on an automated four-circle diffractometer with Mo-K_α radiation.‡

The structure was solved by the heavy-atom method and the positional and thermal parameters were refined by the least-squares method using anisotropic temperature factors for non-hydrogen atoms. The final R value for the 3763 reflexions used in the refinement is 0·060. The absolute configuration of the molecule was determined by anomalous scattering technique.

The resulting molecular structure of the thallium salt of carriomycin, viewed along *b* axis, is shown in the Figure which correctly represents the absolute configuration of the antibiotic. The metal cation is surrounded by the anion and the whole molecule takes a cyclic conformation by a strong hydrogen bond between the hemiacetal hydroxy group of the terminal F-ring and one of the oxygens of the carboxylic group. Interactions between the thallium atom and the oxygens are $< 3{\cdot}0$ Å.

Carriomycin is one of the six polyether antibiotics which were shown to contain a sugar unit in the molecule and its aglycone part is closely related to lonomycin.[11]

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‡ The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Rd., Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication.

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