

The Crystal and Molecular Structure of the Silver Salt of Lysocellin, a New Polyether Antibiotic

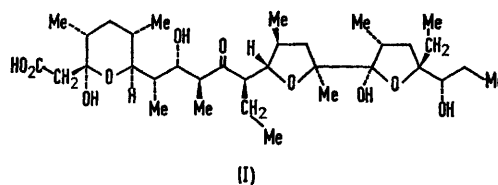
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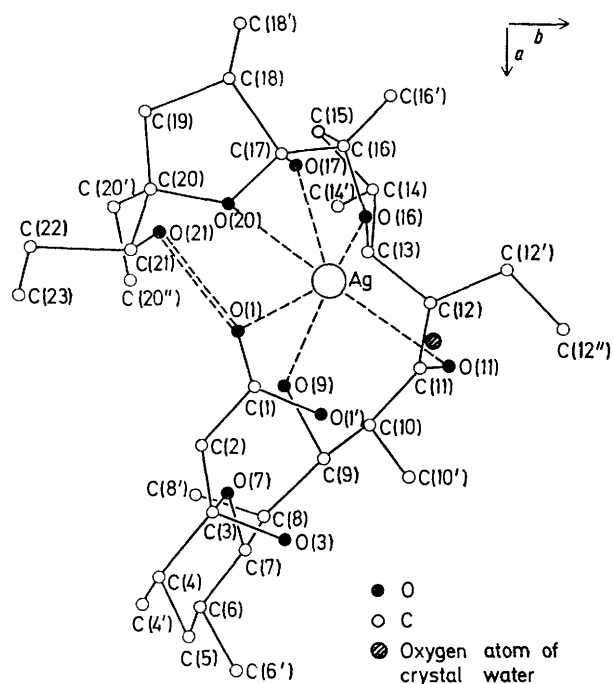
Summary The molecular structure of the antibiotic lysocellin has been established from the crystal structure of the silver salt, $C_{34}H_{59}O_{10}Ag \cdot \frac{1}{2}H_2O$.

LYSOCELLIN¹ is a new antibiotic from *Streptomyces cacaoi* var. *asoensis* which shows antibacterial activity against gram-positive bacteria, mycobacteria and fungi, and is also effective in the treatment of coccidial infections in poultry.

From its biological activity and physicochemical properties lysocellin was assumed to belong to the polyether antibiotics including monensin,² X-537A,³ A2O4A⁴ and salinomycin.⁵

Lysocellin is a monocarboxylic acid existing as an amorphous powder, ν_{max} ($CHCl_3$) 1725 cm^{-1} , pK_a 6.6 (66% dimethylformamide), and forms a crystalline water-insoluble sodium salt, m.p. $158\text{--}160^\circ\text{C}$, $C_{34}H_{59}O_{10}Na \cdot \frac{1}{2}H_2O$





FIGURE

$[\alpha]_D^{25} +11.5^\circ$ (c 1 in MeOH) and a silver salt, $C_{34}H_{59}O_{10}^- Ag \cdot \frac{1}{2}H_2O$, λ_{max} 290 nm (ϵ 3.2×10^4 in MeOH) m.p. $> 123^\circ C$ (decomp.)

The structure of lysocellin was established as (I) by a three-dimensional X-ray structural analysis of the silver salt.

Crystal data: $C_{34}H_{59}O_{10}Ag \cdot \frac{1}{2}H_2O$, space group $P2_12_12_1$, $a = 16.259 \text{ \AA}$, $b = 26.460 \text{ \AA}$, $c = 8.916 \text{ \AA}$, $D_m = 1.18$ (floatation in aqueous NaCl), $D_c = 1.16$, $Z = 4$. 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 the non-hydrogen atoms. The final R value for the 1576 reflexions used in the refinement was 0.070. The absolute configuration of the molecule was determined for the silver salt by anomalous dispersion.

The resulting molecular structure of lysocellin silver salt viewed along the c axis is shown in the Figure which represents the absolute configuration of the antibiotic. The anion is wrapped around the silver. It is held in this conformation by a strong hydrogen bond $O(21) \cdots H \cdots O(1)$ (2.62 \AA , double dotted line) and by interactions between the silver and the six oxygen atoms (single dotted lines): the silver-oxygen distances lie between 2.4 and 3.0 \AA .

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