

Crystal and Molecular Structure of Emericid: a New Polyether Antibiotic

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Summary The molecular structure of the antibiotic emericid has been established from the crystal structure of its silver salt.

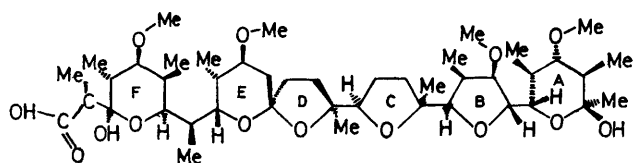
EMERICID is a new antibiotic¹ from *Streptomyces hygrosopicus* DS 24 367 which shows antibacterial activity against gram-positive bacteria and is effective in treatment of coccidial infections in poultry. From its biological activity and physicochemical properties emericid was thought to belong to the family of polyether monocarboxylic acid antibiotics including monensin, nigericin, grisorixin, di-

anemycin, A204, salinomycin, A23187, septamycin, lyso-cellin, alborixin² and X-206.³

The Ag⁺ and Na⁺ salts of emericid are nearly isomorphous. *Crystal data*: Ag⁺ salt; monoclinic, space group $P2_1$, $a = 15.011$, $b = 13.402$, $c = 12.789$ Å; $\beta = 111.3^\circ$, $Z = 2$; $\lambda = 0.7093$ Å; 2365 observed intensities; Na⁺ salt; monoclinic, space group $P2_1$, $a = 14.768$, $b = 13.507$, $c = 12.775$ Å; $\beta = 110.7^\circ$, $Z = 2$; $\lambda = 1.5418$ Å; 3879 observed intensities.

Three-dimensional intensity data were collected with a Philips PW 1100 four-circle diffractometer. The structure

of the silver salt was solved by the heavy atom technique and has been refined to an R value of 12% by least-squares methods using anisotropic temperature factors for the heavy atom and isotropic factors for all other atoms. The



(1)

structure of the sodium salt was refined with anisotropic temperature factors to an R value of 6.1%. The absolute configuration of the molecule was determined from the silver salt by anomalous dispersion with $\text{Cu-K}\alpha$ radiation.

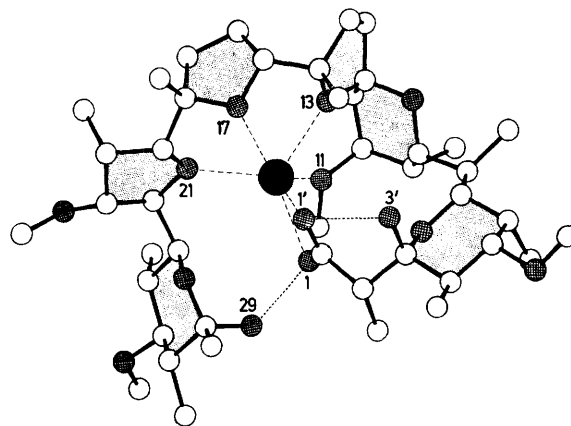
The molecular structure and stereochemistry of the antibiotic emericid is shown to be (1). Ring A is similar in structure and stereochemistry to that in A204A; rings D and E occur in monensin.

TABLE. M-O distances

	Ag	Na		Ag	Na
M-O(1)	2.41	2.38	M-O(13)	2.55	2.40
M-O(1')	2.65	2.45	M-O(17)	2.77	2.51
M-O(11)	2.70	2.50	M-O(21)	2.50	2.45

The structure of the sodium salt of emericid is shown in the Figure. The molecule is wrapped around the cation and held in this conformation by a hydrogen bond (Ag salt: 2.73 Å Na salt: 2.66 Å) between the hydroxyl-group [O(29)]

on ring A and one of the carboxylate oxygen atoms [O(1)], a feature which is usually seen in the crystal structure of polyether antibiotics. The other carboxylate oxygen atom [O(1')] is linked by a strong intramolecular hydrogen bond (Ag salt: 2.63 Å Na salt: 2.63 Å) to the hydroxyl-group on ring F [O(3')].



FIGURE

The cation is co-ordinated to six oxygen atoms. The distances are shown in the Table.

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¹ F. Benazet, J. R. Cartier, J. Florent, C. Johnson, J. Lunel, and D. Mancy, Ninth International Congress of Chemotherapy, London, 1975, abstract M432.

² M. Alleaume, B. Busetta, C. Farges, P. Gachon, A. Kergomard, and T. Staron, *J.C.S. Chem. Comm.*, 1975, 411, and reference therein.

³ J. F. Blount and J. W. Westley, *J.C.S. Chem. Comm.*, 1975, 533.