Crystal Structure of a Barium Complex of Antibiotic X-537A, $Ba(C_{34}H_{53}O_8)_2{\cdot}H_2O$

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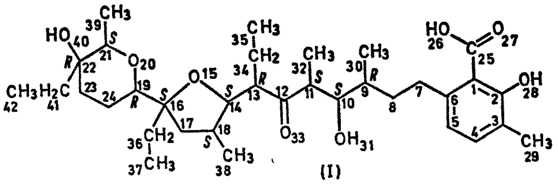
Summary The molecular structure of the antibiotic X-537A has been determined from the crystal structure of a barium salt, $(C_{34}H_{53}O_8)_2Ba{\cdot}H_2O$.

RECENT interest[1,2] in polyether antibiotic acids stimulated a crystallographic investigation of a derivative of the antibiotic X-537A, which was originally isolated in 1951 from an unidentified Streptomyces.[3] The complex of two molecules of the monovalent anion of X-537A with Ba^{2+} formed crystals suitable for X-ray analysis. Crystal data: $Ba(C_{34}H_{53}O_8)_2{\cdot}H_2O$, M 1334·9, monoclinic, $a = 14{\cdot}59(4)$, $b = 17{\cdot}95(5)$, $c = 13{\cdot}99(4)$ Å, $\beta = 105°17'(15')$, $U = 3534{\cdot}1 \times 10^{-24}$ cm^3 $D_m = 1{\cdot}22$, $D_c = 1{\cdot}255$ g cm^{-3}, $Z = 2$, space group $P2_1$.

The structure determination, although complicated by the pseudosymmetry resulting from one heavy atom in the asymmetric unit of the space group $P2_1$ and by the lack of chemical information about the molecular structure, was achieved by the heavy-atom method. The structure has been refined to an R-factor of 0·11 on 4753 structure amplitudes collected by visual estimates from photographic film using Cu-K_α radiation.



(I)

A stereoscopic view of the complex is shown in Figure 1, from which it is seen that the antibiotic X-537A has the structure (I). [The atom numbering system used in the Figures and in structure (I) is arbitrary and does not correspond to any chemical convention.] Subsequent chemical evidence[2] indicated that the absolute configuration is as depicted in (I). The crystal consists of discrete,

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$Ba(C_{34}H_{53}O_8)_2{\cdot}H_2O$ units with no inter-complex hydrogen-bonding. The barium ion is closely approached by nine oxygen atoms, with $Ba^{2+}\cdots O$ distances ranging from 2·71—3·08 Å. Six oxygen atoms from one antibiotic anion, two from the other anion, and the water molecule of crystallisation co-ordinate to the metal ion. A detailed view of the co-ordination of barium is shown in Figure 2. Despite the different modes of co-ordination to barium and the location of a water molecule close to one of the antibiotic anions, the molecular conformations of the two anions are remarkably similar. The circular conformation of the anion is largely dictated by "head" to "tail" hydrogen bonding, O(40)–H···O(26). A somewhat similar circular conformation, apparently stabilized by "head" to "tail" hydrogen bonding, is observed in the anions of the monensin[1] and nigericin[4,5] antibiotics.

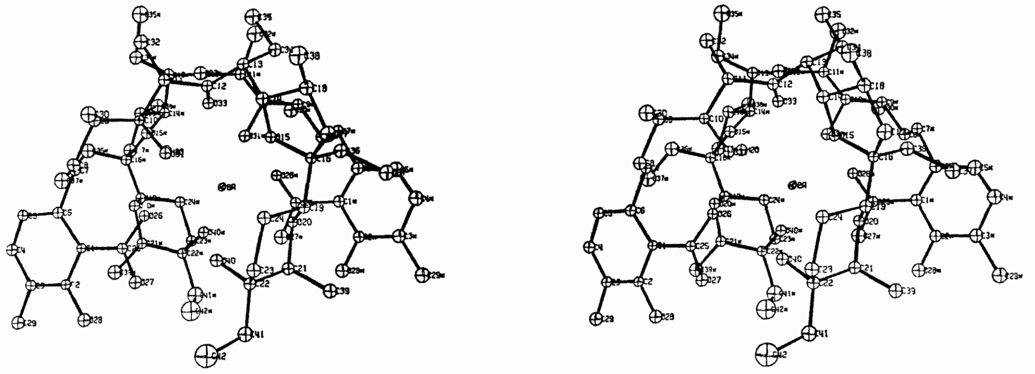

FIGURE 1. *Stereoscopic picture of the complex viewed along the* x *axis.*

The two X-537A anions effectively "sandwich" the Ba^{2+} ion and, as almost all the oxygen atoms are directed towards the centre of the complex, afford a protective hydrophobic exterior which undoubtedly accounts for the high solubility in non-polar organic solvents and the low solubility in water. Full details of the structure of the complex will be the subject of a forthcoming paper.[6]

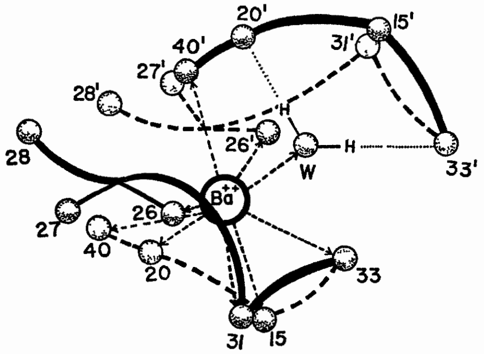

FIGURE 2. *Schematic drawing of the co-ordination of barium. Only the oxygen atoms of the antibiotic molecules are shown.*

(*Received, November 3rd,* 1969; *Com.* 1678.)

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