# The Crystal Structure and Stereochemistry of Laurencin

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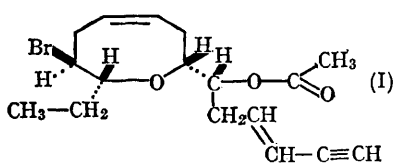
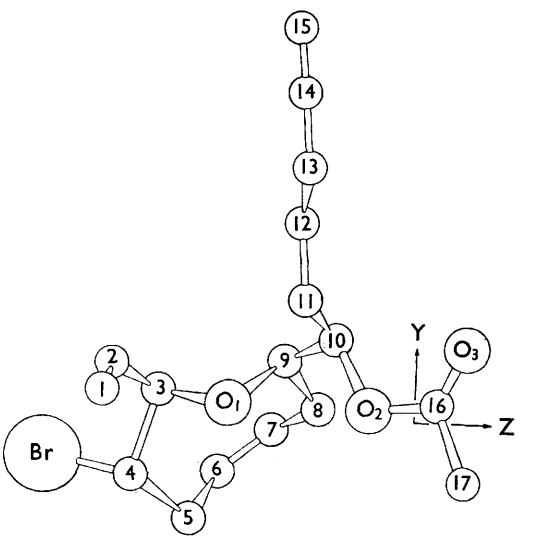
IRIE, SUZUKI, and MASAMUNE[1] have described a naturally occurring bromo-compound, laurencin, $C_{17}H_{23}O_3Br$, isolated from *Laurencia glandulifera*. From an extensive chemical and spectroscopic investigation they have proposed an eight-membered ring structure, although the possibility of a nine-membered ring could not be completely eliminated, and no details of the stereochemistry, particularly at the four asymmetric centres, are yet available.

We have obtained from Professor Irie some beautiful rock-like crystals of laurencin, and our study of the crystal structure now fully confirms Professor Irie's structural formula, and in addition provides the stereochemistry and dimensions of this interesting molecule. The relative stereochemistry is shown in (I).




(I)

Laurencin crystallises in the orthorhombic system, space group $P2_12_12_1$ with four molecules of $C_{17}H_{23}O_3Br$ in a unit cell of dimensions $a = 7{\cdot}70$, $b = 9{\cdot}70$, $c = 22{\cdot}93$ Å. Some 1150 structure amplitudes were measured on our linear diffractometer,[2] but as the crystals tend to decompose in the *X*-ray beam some errors may exist in the data, which are now being estimated again by photographic methods. The information available, however, is already sufficient to establish the structure, which was solved by the heavy-atom method[3] with initial phasing on the bromine atom. The conformation of the eight-membered ring and the orientation of the exocyclic groups are shown in the figure. The value of $R$ is now 24% and refinement of the atomic parameters is continuing.




FIGURE

*The atomic arrangement in a molecule of laurencin as viewed along the* a*-axis of the crystal.*

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[1] T. Irie, M. Suzuki, and T. Masamune, *Tetrahedron Letters*, 1965, 1091.
[2] U. W. Arndt and D. C. Phillips, *Acta Cryst.*, 1961, **14**, 807.
[3] J. M. Robertson and I. Woodward, *J. Chem. Soc.*, 1937, 219; 1940, 36.