The Structure of Hopeaphenol

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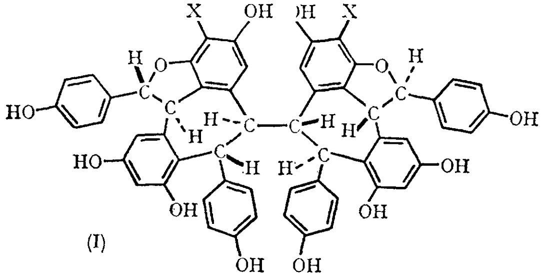
HOPEAPHENOL, which has now been isolated from four members of the family Dipterocarpaceae, was shown by the preliminary work already reported[1] to be a polyhydric phenol of high molecular-weight and apparently chemically unrelated to other natural phenols. We have recently been able to prepare a crystalline dibromo-derivative of the decamethyl ether of hopeaphenol and have determined its structure by *X*-ray methods.

The dibromide, which crystallises from benzene-methanol as a benzene solvate, has the monoclinic space group *C*2 with four units of $C_{66}H_{60}O_{12}Br_2$,-$2C_6H_6$ per unit cell. The lattice parameters are $a = 21{\cdot}75$, $b = 11{\cdot}31$, $c = 27{\cdot}78$ Å, $\beta = 95{\cdot}42°$.

The intensities of 2,870 independent reflections were measured on an Arndt–Phillips linear diffractometer using Mo-K_α radiation. The positions of the bromine atoms, as found from the three-dimensional Patterson synthesis, were refined using the structure factor least-squares programme written by Dr. R. Diamand. The rest of the structure emerged from five successive three-dimensional electron-density Fourier syntheses. Refinement of the atomic positions and isotropic temperature factors by least squares reduced the *R*-factor to 0·17 for all observed reflections. The bond lengths and angles are satisfactory at this stage of the refinement and the stereochemistry is apparent. In addition to the structure of the phenol derivative it has now become possible to find the position of the benzene solvate molecules in the lattice and refinement is continuing taking these positions into account and using anistropic temperature factors for the bromine atoms.

It is known that the preparation of the dibromide does not involve a rearrangement so the structure of this derivative revealed by the *X*-ray analysis enables the structure of hopeaphenol itself to be derived. This is indicated in the formula (I) which shows the relative stereochemistry of the asymmetric centres. In the bromo-derivative of the ether the halogen atoms occupy the positions designated X in the formula.



(I)

The structure of hopeaphenol is of a unique type but formally it can be regarded as made up of four units of 3,5,4-'trihydroxystilbene (resveratrole) and it is tempting to assume that hopeaphenol is biosynthesised from this precursor or from a similar molecule by oxidative processes, even though stilbenes have not yet been reported as occurring in any of the Dipterocarpaceae.

The crowded nature of the molecule of hopeaphenol and its simple derivatives has interesting effects on the nuclear magnetic resonance frequencies of some of its hydrogen nuclei. Some, but not all, of these anomalous absorptions can be simply rationalised in terms of long-range shielding by the benzene rings.

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[1] P. Coggon, N. F. Janes, F. E. King, T. J. King, R. J. Molyneux, J. W. W. Morgan, and K. Sellars, *J. Chem. Soc.*, 1965, 406.