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ISOLATION OF 3,3′,4′,5,5′-PENTAHYDROXYSTILBENE FROM *SCHOTIA* SPECIES

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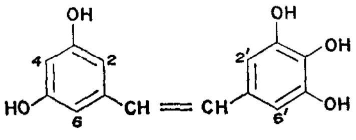
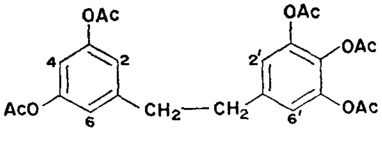
Abstract—3,3′,4′,5,5′-Pentahydroxystilbene has been isolated in exceptionally high yield from the heartwood of *Schotia brachypetala.*

METHANOLIC extraction of the dark red heartwood of *Schotia brachypetala* (Leguminosae) has afforded 3,3′,4′,5,5′-pentahydroxystilbene (I) in high yield (7·2% on wood weight). This stilbene has not previously been isolated in the free phenolic form from natural sources. King *et al.*[1] first obtained it as a mixture with 3,3′,4′,5-tetrahydroxystilbene from the wood of *Vouacapoua macropetala* and were able to separate it as the pure pentaacetate. Hydrolysis of the latter then gave the free phenol. Hillis[2] has presented paper chromatographic evidence for the likely presence of this pentahydroxystilbene in the heartwood of *Eucalyptus astringens.*



I



II

The structure of the polyphenol was established by degradation with KOH, coupled with NMR and mass spectrometric analysis of derivatives. In common with other stilbenes, the compound has an intense fluorescence in UV light with maxima at 225 and 325 nm. The NMR spectrum of the stilbene is shown in Fig. 1. The dimethylsulphoxide used as solvent proved to be particularly suitable since the pattern of substitution of the aromatic rings is clear, the phenolic groups are readily discernable downfield and there is no overlap from the methyl groups of the solvent itself. The crystalline pentaacetate had M^+ 470 and the mass spectrum illustrated clearly the successive loss of five phenolic acetyl groups. Final proof of structure was obtained from hydrogenation of the stilbene with PtO_2 in methanol. This gave the pentahydroxydibenzyl derivative which on acetylation yielded the crystalline pentaacetate II, m.p. 123°, M^+ 472. The NMR spectrum exhibited the two methylene groups as a singlet at τ 7·13.

The 3,3′,4′,5,5′-pentahydroxystilbene (assumed to be the *trans* compound[3]) although white initially, rapidly turns yellow on exposure to sunlight or on being heated above 100°.

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[1] F. E. KING, T. J. KING, D. H. GODSON and L. C. MANNING, *J. Chem. Soc.* 4477 (1956).

[2] W. E. HILLIS and A. CARLE, *Biochem. J.* 82, 435 (1962).

[3] G. BILLEK, in *Progress in the Chemistry of Organic Natural Products* (edited by L. ZECHMEISTER), p. 115, Vol. 22, Springer, New York (1964).

Stilbenes are known to undergo cyclizations[4] and photodimerizations[5] and this behaviour of the compound is under investigation.

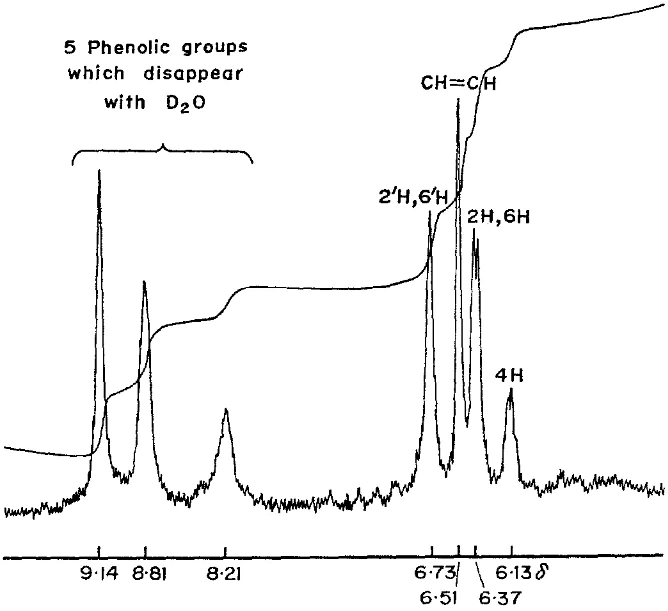

FIG. 1. NMR SPECTRUM OF 3,3',4',5,5'-PENTAHYDROXYSTILBENE IN DIMETHYLSULPHOXIDE.

EXPERIMENTAL

Isolation. Fresh heartwood drillings (1·5 kg) from a mature trunk of *Schotia brachypetala* were extracted with methanol (10 l.) for 5 days (room temp.). Evaporation of the solvent under vacuum to a small volume (1·5 l.) followed by dilution with water (to 2 l.) gave white clusters of prisms (108 g) m.p. 245° (lit.[1] 245°). (Found: C, 65·09; H, 5·04. Calc. for $C_{14}H_{12}O_5$: C, 64·61; H, 4·65%). The compound is insoluble in water. It exhibits dark brown and orange-red colours when sprayed with ammoniacal silver nitrate and diazotized benzidine respectively.

Degradation. Microfusion[6] with KOH showed the presence of resorcinol and pyrogallol. The identity of these products was proved by co-chromatography with authentic reference compounds.

Preparation of derivative. The stilbene (250 mg) was acetylated with pyridine/Ac_2O for 10 hr at room temp. The derivative (260 mg) was recovered from water and recrystallized from methanol, m.p. 173° (lit.,[1] 173–174°). (Found: C, 60·92; H, 4·71. Calc. for $C_{24}H_{22}O_{10}$: C, 61·27; H, 4·72%).

Hydrogenation. Stilbene (700 mg) in methanol (50 ml) was hydrogenated over PtO_2 (100 mg) for 4·5 hr. The product failed to crystallize and was then acetylated as above. From ethanol white prisms (200 mg) m.p. 123°, were obtained. (Found: C, 60·75; H, 5·12. $C_{24}H_{24}O_{10}$ required: C, 61·01; H, 5·12%).

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[4] H. GÜSTEN and L. KLASINC, *Tetrahedron* **24**, 5499 (1968).

[5] H. ULRICH, D. V. RAO, E. A. STUBER and A. A. R. SAYIGH, *J. Org. Chem.* **35**, 1121 (1970)

[6] D. G. ROUX *J. Amer. Leather Chemists' Assoc.* **53**, 384 (1958).