Tetrahedron Letters No.46, pp. 5727-5730, 1966. Pergamon Press Ltd.
Printed in Great Britain.

THE STRUCTURE OF MESUOL

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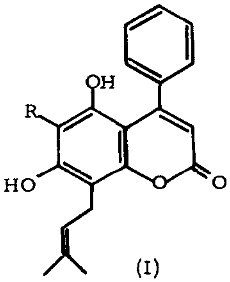
(Received 31 August 1966)

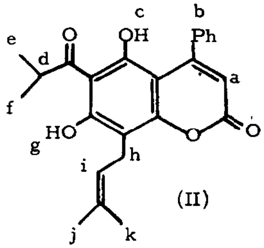
Mesuol, m.p. 154°, an optically inactive pale-yellow crystalline bitter antibiotic (1), isolated from Mesua ferrea Linn., was assigned the molecular formula $C_{23}H_{22}O_5$ by Dutta et al. (2). Chakraborty and Bose (3) obtained acetophenone, phloroglucinol and isovaleric acid by alkali fusion of mesuol. On the basis of the previously reported molecular formula and the results of degradation obtained by them, mesuol was partially formulated as (I). The molecular formula has now been revised to $C_{24}H_{24}O_5$ on the basis of the mass spectral data of mesuol ($M^+ = 392$) and its dimethyl derivative ($M^+ = 420$). The present communication relates to further studies which establish the structure of mesuol as (II).

It appears from the N.M.R. data (the N.M.R. assignments of the protons are shown below the appropriate formula) and previously obtained results (3), that mesuol contains a 5,7-dihydroxy 4-phenyl coumarin skeleton with an isopentenyl chain and a C_4H_7O fragment present as an isobutyryl chain. The presence of a band at 1697 cm^{-1} in the I.R. spectrum of dimethyl mesuol (which is

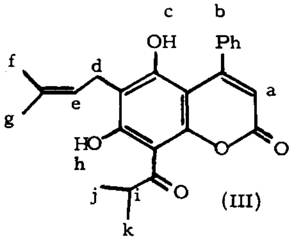


(I)

R = C_3H_5O



(II)



(III)

a	τ	4.08 (1H) s.
b		2.52 (5)
c		- 0.94 (1) s.
g]		0.36 (1) s.
d		6.25 (1) m.
e f]		8.90 (6) d. *J* 7 c/s
h		6.45 (2) d. *J* 7 c/s
i		4.72 (1) m.
j]		8.12 (3) s.
k]		8.25 (3) s.

a	τ	3.92 (1) s.
b		2.40 (5)
c		4.01 (1) s.
d		6.65 (2) d. *J* 7 c/s
e		4.84 (1) m.
f g]		8.30 (6) broad s.
h		-4.70 (1) s.
i		6.10 (1) m.
j k]		8.70 d. *J* 7 c/s

absent in the I.R. spectrum of mesuol) indicates that the acyl function is chelated. Both the hydroxyl groups of mesuol are also chelated to the acyl function as evidenced by the presence of two hydroxyl protons (disappear on deuteration) at τ - 0.94 and 0.36 (4). These data suggest the location of the isobutyryl residue at position 6 of the coumarin nucleus. Consequently, the isopentenyl group should occupy position 8, as was assumed by Chakraborty and Bose (3).

Mesuol on treatment with 5 % methanolic or with 10 % aqueous potassium hydroxide was isomerised to isomesuol (M^+=392) (III), $C_{24}H_{24}O_5$, m.p. 171°. This isomerisation is parallel to that observed in the case of mammea A/BA to A/AA (4). N.M.R. data of isomesuol (III) show that one of the two hydroxyls (τ -4.70 and 4.01 ; disappear on deuteration) is, as expected, chelated to the acyl carbonyl. On degradation with 40 % aqueous potassium hydroxide mesuol furnished acetone, acetophenone, isovaleric acid and a compound $C_{20}H_{18}O_4$, m.p. 268°, which is a 4-phenyl coumarin derivative [I, R = H ; Lit. m.p. 214°(5)]. Dimethyl mesuol is stable toward 40% aqueous alkali. These results are in agreement with the structure (II) for mesuol.

Though recently butyryl side chain has been encountered in the coumarin series (4), the isobutyryl side chain in a coumarin has been found for the first time in mesuol. Some naturally occurring ketones built on phloroglucinol units have isobutyryl residue linked with the aromatic nucleus (6).

Acknowledgement :

We thank Dr. D.M. Bose, Director, and Dr. A. Sen, Head of the Department of Chemistry, Bose Institute, for their interest in this work. We also express our gratitude to Dr. P.K. Bose for his keen interest in this problem.

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