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TERPENOIDS LXXXIX

ABSOLUTE CONFIGURATION OF PARTHENOLIDE*

A.S. Bawdekar, G.R. Kelkar and
S.C. Bhattacharyya
National Chemical Laboratory, Poona, India.

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The sesquiterpenic lactone, parthenolide, isolated from Chrysanthemum parthenium (L) Bernh, was previously assigned the structure I, by Sorm and co-workers.[1] Recently Govindachari et al[2] isolated the same compound from the trunk bark of Michelia champaca and revised its structure to II from a study of its NMR spectrum and chemical reactions. However, the stereochemistry of the molecule at the various centres does not appear to have been established so far. We are now able to show that parthenolide can be represented by the stereoformula III and dihydroparthenolide by IV.

Parthenolide has a close structural similarity with costunolide (V) and dihydrocostunolide (VI; m.p.77-78°), stereochemistry of both of which is well established.[3] Parthenolide can be considered as the 4,5-monoepoxide of costunolide and dihydroparthenolide the 4,5-monoepoxide of dihydrocostunolide.

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Attempts to prepare the mono and diepoxides of costunolide (V) in the pure form were unsuccessful, due to simultaneous formation of several closely related products and polymerisation. Mono-epoxidation of dihydrocostunolide (VI), preferentially at one of the double bonds also could not be achieved, though the course of reaction was carefully followed by suitable rate study. Addition of calculated amount of perbenzoic acid under controlled conditions gave a product which analytically corresponded to a monoepoxide, but was actually a mixture of several products (TLC) from which chromatography or crystallisation did not lead to any pure isolate.

However, dihydrocostunolide (VI; m.p. 77-78°; $(\alpha)_D$ + 113.6°) yielded on treatment with excess of perbenzoic acid (2.2 moles) in chloroform solution (96 hr), a crystalline diepoxide, $C_{15}H_{22}O_3$* (VII), m.p. 160-65°, which after crystallisation from benzene-petroleum ether melted at 172-73°; $(\alpha)_D^{27}$ - 66.43° ($CHCl_3$; c, 5.7). It was identical with the epoxide of dihydroparthenolide as established by comparison of the IR and NMR spectra and mixed melting point with an authentic sample kindly supplied by Prof. Govindachari.

The stereochemistry of parthenolide at C_6 and C_7 and that of dihydroparthenolide at C_6, C_7 and C_{11} is thus established.

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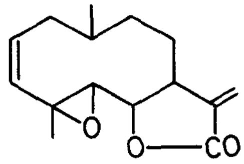
* All the compounds gave satisfactory elemental analyses.



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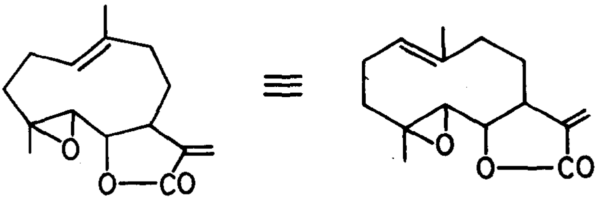

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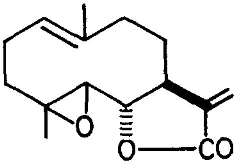

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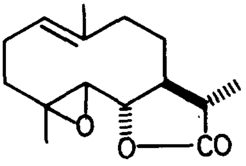

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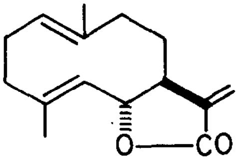

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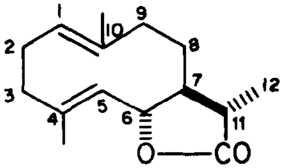

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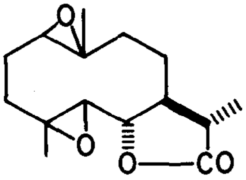

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