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AN UNUSUAL HYDROCARBON

by

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AN UNUSUAL triterpenoid hydrocarbon, botryococcene ($C_{34}H_{58}$), constitutes ~70% of the dry weight of the brown resting state of the alga *Botryococcus braunii*[1]. This colourless oil is of interest because of the large quantity in which it is produced by *B. braunii* and the possibility of its future use as a precursor of organic intermediates and fuels of commercial significance[2]. The alga, *B. braunii*, occurs in a variety of climates in Asia, Australia, America, New Zealand and Scandinavia. It is common, but not abundant, in Britain. Usually it is found in fresh water but occurs also in the salt water of Lake Balkhash (Central USSR). Colonies of the alga vary in size, texture and structure; and at least three physiological states have been distinguished by light microscopy and hydrocarbon content. In only one of these is botryococcene present as the major hydrocarbon.

To examine possible future uses of this compound investigation of its structure was required. Preliminary work was thus carried out by Maxwell *et al*[3] and furthered by Cox[1] and co-workers[4]. Chromatographic separation of acetone extract of freeze-dried *B. braunii* afforded a pure sample of botryococcene. On the basis of infrared, ^{1}HNMR, ^{13}CNMR, mass spectroscopy, hydrogenation, oxidative degradation and established biosynthetic principles, structure I was proposed for botryococcene[1,4].

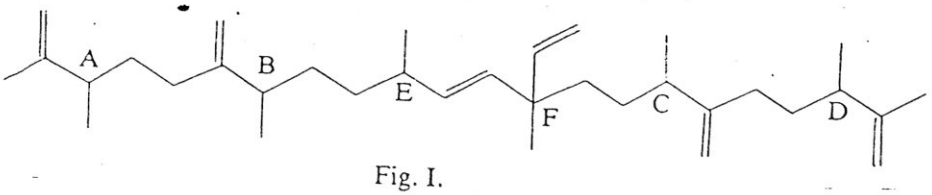

Fig. I.

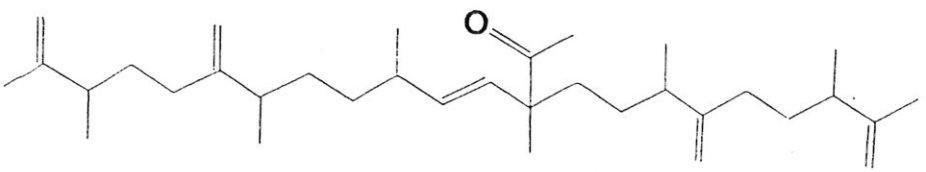

Fig. II.

Botryococcene (I) has six chiral centres (carbons A, B, C, D, E and F), the configuration about these not being known. A study[3] was undertaken to determine the stereochemical configuration of

this compound, and two possible approaches were investigated: (i) preparation of a crystalline derivative of the compound, suitable for X-ray crystallographic analysis; and (ii) oxidative cleavage of the molecule to smaller fragments each with one or two chiral carbons and optical rotation studied on these. The earlier of the two approaches is complicated by the fact that botryococcene is difficult to form into suitable solid derivatives without affecting its stereochemistry at one or more points in the molecule. It therefore became necessary to convert botryococcene into some other, easier to derivatise, molecule without altering the main carbon chain in any way. Botryococcene (I) was thus converted to an entirely new compound, botryococcone (II) (a methyl ketone), using a highly specific oxidation of vinyl double bond in botryococcene[2]. Formation of solid derivatives of this compound has so far not been achieved. Investigation continues, however.

The second approach of oxidative cleavage was attempted[1,2] using several different (permanganate, permanganate-periodate, ruthenium tetroxide, etc.) oxidations. Two-phase systems were used due to the hydrophobic nature of botryococcene and aqueous requirement of oxidation reactions. In all cases small yields and high complexity of product mixtures made further study difficult. Attempts to increase the yield of these oxidations using phase transfer agents[2] and chelating molecules[2] have not been very promising. Biological oxidation of botryococcene using certain strains of yeasts also proved unsuccessful[1]. The possibility of directly incorporating botryococcene into the crystals of certain sulphur-containing organic compounds is now being experimented with. The aim once again is to use these crystals for X-ray diffraction studies[5]. Other possible approaches are being actively pursued elsewhere in the world. So far, however, this interesting problem of organic chemical structure remains to be fully solved.

A complete knowledge of the structure of botryococcene will be helpful in understanding its exact biosynthetic pathway in the parent alga and this in turn will permit an improvement in the yield of this compound. With rising oil prices coupled with foreseeable shortages, commercial extraction of botryococcene might become desirable!

References

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