Confirmation of the Structure of Thujic Acid by Nuclear Magnetic Resonance

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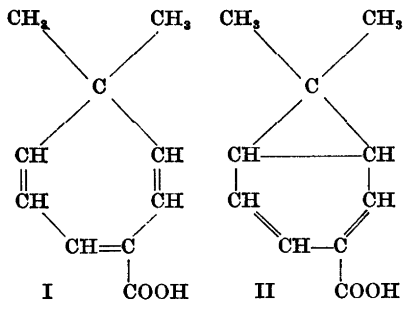
In a previous paper [1] it was pointed out that there are two likely structures for thujic acid, namely (I) and (II).



Degradation and synthesis [1,2] were definitely in favour of (I), which has therefore been regarded as the correct structure of thujic acid.

Confirmation of this structure by some independent means, preferably by a method not involving chemical reactions appeared, however, to be very desirable. Corey *et al.*[3] have recently solved a similar problem in the eucarvone series by the use of nuclear magnetic reasonance [4].

Dr. J. N. Shoolery of Varian Associates has been kind enough to measure the N M R spectrum of thujic acid methylester, which is reproduced in Fig. 1.

The shift in resonance is expressed as mgauss relative to benzene as zero standard, with an applied magnetic field of 7 050 gauss. There are three different bands of absorption. The very complex one at A is due to the ethylenic hydrogens. The sharp peak at B is due to the ester methyl group, while the *gem*-dimethyl hydrogens absorb at C. There is no absorption at about 35 mgauss, where the tertiary bridge hydrogens of (II) should absorb [3]. Furthermore the area under A is close to that under C, but much greater than that under B, which is also in agreement with structure (I) with five ethylenic hydrogens.

There is thus no doubt that (I) correctly represents thujic acid.

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1. Gripenberg, J. *Acta Chem. Scand.* **5** (1951) 995.
2. Gripenberg, J. *Acta Chem. Scand.* **3** (1949) 1137.
3. Corey, E. J., Burke, H. J. and Remers, W. A. *J. Am. Chem. Soc.* **77** (1955) 4941.
4. Purcell, E. M. *Science* **118** (1953) 431.

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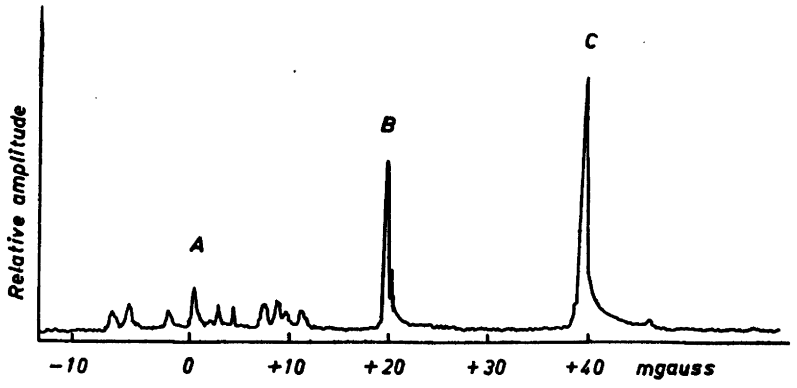

Fig. 1.