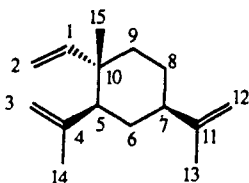


Rebuttal on Sesquiterpene Composition of Basil Oil. Assignment of the ^1H and ^{13}C NMR Spectra of β -Elemene with Two-Dimensional NMR

Sir: The argument of Brauchli and Thomas concerning the ^1H and ^{13}C assignments of β -elemene [We have taken, in this letter, the numbering of secoeudesmanes, like Brauchli and Thomas, for β -elemene. Our previous numbering (Gaydou et al., 1989) was in relation to structure determination.] starts from the fact that we have made an error in the observation of a "zigzag coupling" between H-2a and H-5 in the ^1H NMR spectrum (Gaydou et al., 1989).



Brauchli and Thomas realize the ^1H NMR assignments of the two methinic protons H-5 and H-7 using their splitting pattern. This attribution has been confirmed by correlation peaks observed between these two methinic protons and the isopropylidene group.

As shown in Figure 1, one can note, in our case, a diagonal peak between a methinic proton and the $\text{CH}_2=\text{CH}$ group which can be interpreted as a zigzag coupling between H-2a and H-5. A homonuclear J -resolved experiment (Figure 2) allowed us a fine determination of the coupling figure of this proton system H-5 and H-7. Taking into

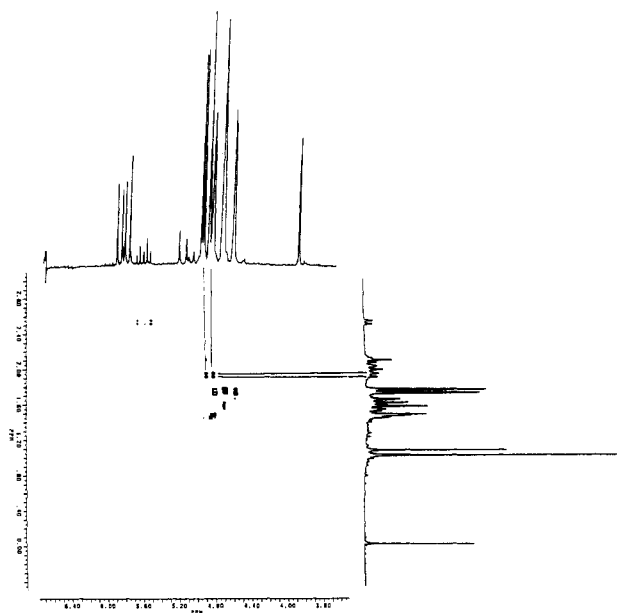


Figure 1. Ethylenic part vs aliphatic part of the COSY spectrum of β -elemene, showing the cross peaks between H-2a and H-5.

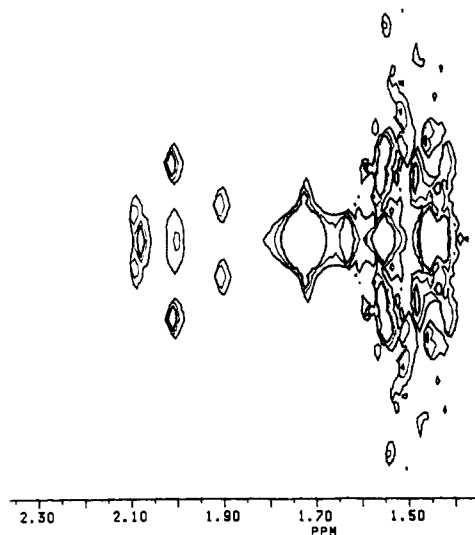


Figure 2. Median part of the 2D J -resolved homonuclear correlation for β -elemene.

account this response, we agreed with the Brauchli and Thomas observation concerning the proton at 2.01 ppm, but we find that the proton at 1.91 ppm (1.94 ppm for Brauchli and Thomas) corresponds to a diffuse doublet and not to a complex multiplet as observed by these authors. Our coupling pattern, on the monodimensional spectrum, of the methyl groups is complex since the couplings between the methylenic group and the methinic protons H-5 and H-7 are shown.

We have not observed correlation peaks between methylenic protons of isopropylidene groups and methinic protons H-5 and H-7. This problem lies open, and an elegant means of finding an answer is probably to realize COLOC or HMBC experiments.

LITERATURE CITED

- Gaydou, E. M.; Faure, R.; Bianchini, J. P.; Lamaty, G.; Rakotonirainy, O.; Randriamiharisoa, R. P. Sesquiterpene Composition of Basil Oil. Assignment of the ^1H and ^{13}C NMR Spectra of β -Elemene with Two-Dimensional NMR. *J. Agric. Food Chem.* 1989, 37, 1032-1037.

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