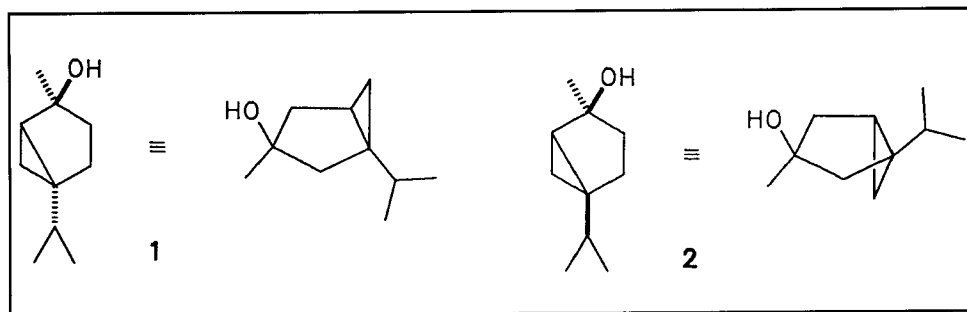


cis- and trans-Sabinene Hydrate: Comparisons of Quadrupole and Ion Trap Mass Spectra

Received: February 1991

Revised: December 1991

The assigning of stereochemistry to the sabinene hydrates is confusing due to the differences between classical terpenoid, modern, preferred and the Chemical Abstracts Service (CAS) nomenclature. For example, Erman (1) elucidates the nomenclature for compound [1] as Classical: trans-sabinene hydrate; Correct: cis-sabinene hydrate; and Preferred: cis-thujan-4-ol. Whereas Erman's 'Correct' terpenoid nomenclature refers to the 'cis-' relationship between the methyl and isopropyl groups, CAS uses a naming hierarchy in which the alcohol (-OH) group takes precedence over the methyl group. Thus, CAS treats [1] as trans- because of the hydroxy (2.beta) and isopropyl groups (5.alpha). Undoubtedly, this has led to numerous errors in assigning registry numbers in published papers and the user of the data bases should be very careful in assuming that computer searches will retrieve the desired isomer.



cis-Sabinene Hydrate [1]:

CAS No. 15826-82-1

MF C10 H18 O FW 154 DB5-629

CN Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-(1.alpha, 2.beta, 5.alpha)(9CI)

Synonym: cis-4-thujanol

trans-Sabinene Hydrate [2]:

CAS No. 17699-16-0

MF C10 H18 O FW 154 DB5-560

CN Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-(1.alpha, 2.alpha, 5.alpha)

(9CI)

Synonym: trans-4-thujanol

Libbey and Sturtz (2) pointed out that "faulty spectra" of cis- and trans-sabinene hydrate were encountered in most of the mass spectral collections. Because the stereochemistries of cis- and trans-sabinene hydrates were confirmed by ^1H NMR in *Strobilanthes callosus* (3), we can now present mass spectra of the isomers on both quadrupole and ion trap mass spectrophotometers and show some of the variation expected from mass spectrophotometers for these compounds.

The quadrupoles gave somewhat different spectra and this appears to be due to the amount of material ionized (or the position in the peak). Notice that quadrupoles #2 and #3 are pretty similar as are quadrupoles #1 and #3 (when the spectrum is taken with 565,284 ions). Apparently the quadrupole mass spectrophotometers give an abundance of the 71 ion when overloaded. It is worth noting that the spectrum in the EPA/MSDC data base (5) has the large 93 ion as with quadrupoles #2 and #3 (with 15,472 ions).

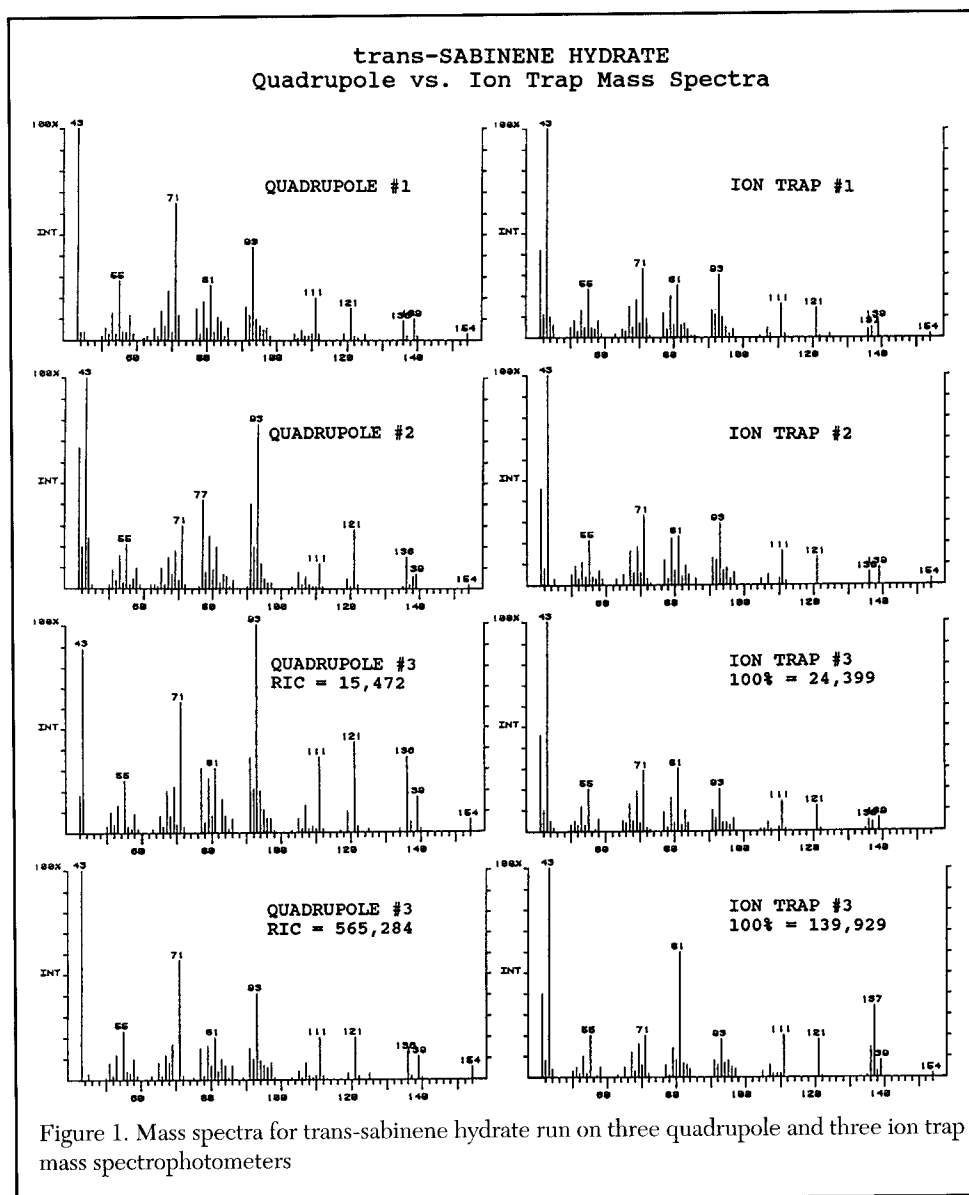


Figure 1. Mass spectra for trans-sabinene hydrate run on three quadrupole and three ion trap mass spectrophotometers

The three ion traps gave very similar spectra but one should note that overloading is a very severe problem on ion traps also. Notice ion trap #3, with 100% = 139,929 ions, has large 81 and 137 ions.

Very similar results were obtained for cis-sabinene hydrate (Figure 2). Because the same sample of *Strobilanthes* oil was run on DB5 (=SE 54) columns on both the ion trap and quadrupole instruments, with very comparable retention indices, it is unlikely that the observed differences are due to a co-eluting compound. Furthermore, single ion searches and consecutive spectra through the cis-sabinene hydrate peak indicated the peak was pure. These ion trap spectra for ion trap #3 (100% = 20,866) should be substituted for those in [4, p. 243, 244] and the retention times on DB5 changed to 560 (trans-) and 629 (cis-) sec. as the trans-elutes before the cis-isomer on DB5.

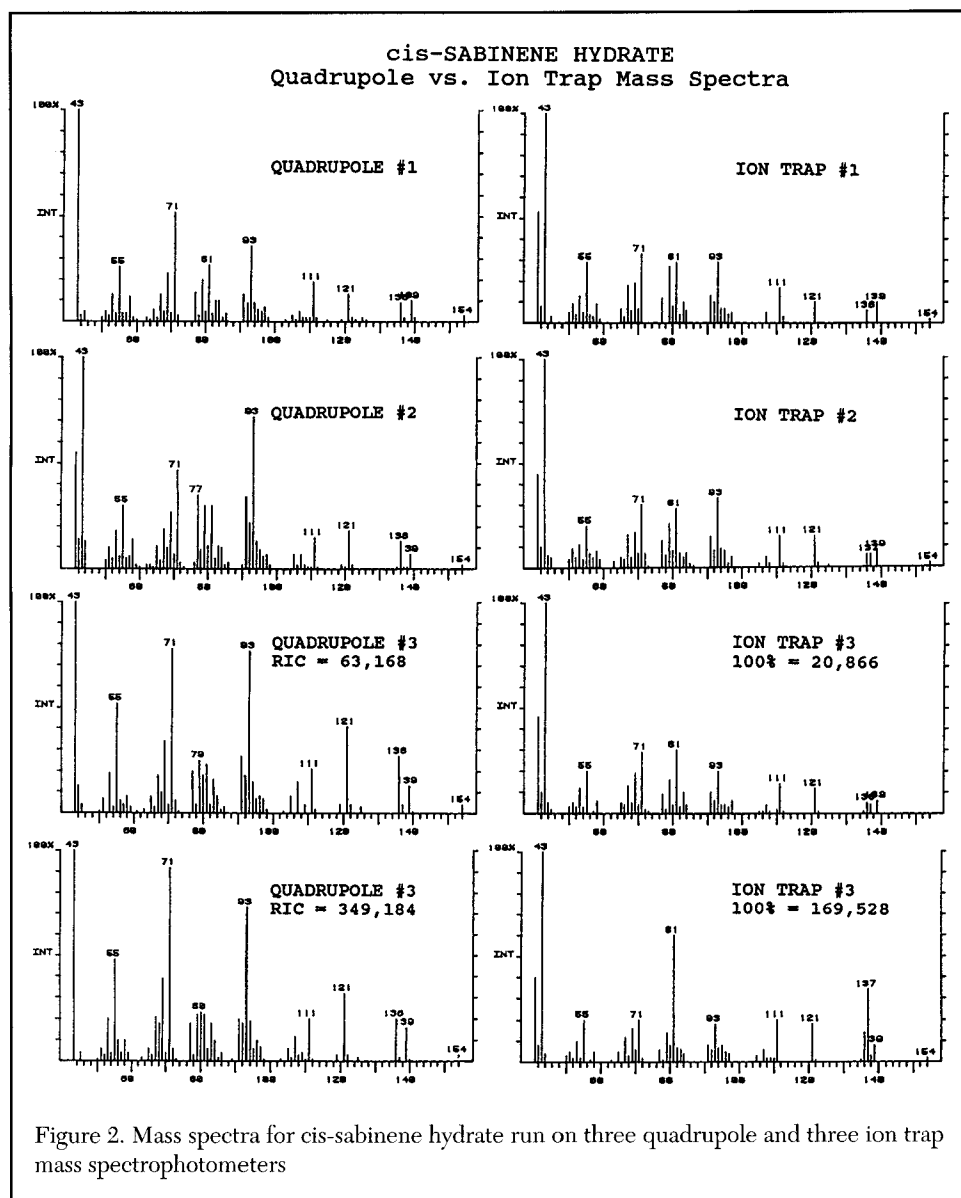


Figure 2. Mass spectra for cis-sabinene hydrate run on three quadrupole and three ion trap mass spectrophotometers

There appears to be no "correct" spectrum for the sabinene hydrates on either quadrupole or ion trap mass spectrophotometers but one can get very reproducible spectra by avoiding overloading.

Instruments used: Quadrupole #1: HP5970 MSD; #2: Varian-Mat 44S; #3: Finnigan 4000. Ion trap #1: Varian Saturn; #2: Finnigan ITD 800; #3: Finnigan ITD 800.

ACKNOWLEDGMENTS: This research was supported in part with funds from the Helen Jones Foundation. Thanks to Drs. Rick Estell, Lawrence Hogge, Tom Phillips and Art Tucker for running the sample on their systems.

REFERENCES

1. W. F. Erman, *Chemistry of the Monoterpenes. Part B.* Marcel Dekker, New York (1985).
2. L. M. Libbey and G. Sturtz, *Unusual Essential Oils Grown in Oregon. III. Thymus 'Pinewood.'* J. Essent. Oil Res., **2**, 193-195 (1990).
3. P. Weyerstahl, H. Marschall-Weyerstahl, V. K. Kaul, E. Manteuffel and L. Glasow, *Constituents of the essential oil of Strobilanthes callosus.* J. Essent. Oil Res. (in press).
4. R. P. Adams, *Identification of Essential Oils by Ion Trap Mass Spectroscopy.* Academic Press, New York (1989).
5. S. R. Heller and G.W.A. Milne, *EPA/NIH Mass Spectral Data Base.* US Government Printing Office, Washington, DC (1987, 1980, 1983).

R. P. Adams
Plant Biotechnology Center
Baylor University
Box 7372
Waco, TX 76798

P. Weyerstahl
Institut für Organische Chemie
Technische Universität Berlin
Strasse de 17 Juni 135
D-1000 Berlin 12, Germany