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Thermochemical properties of sesquiterpenes in natural products by correlation gas chromatography: Application to bergamotene oil

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Abstract:

The vapor pressures and vaporization enthalpies of the three major components of bergamotene oil have been evaluated by correlation gas chromatography. Three major components were identified by GCMS as *E* β -caryophyllene, *trans* α -bergamotene and α -humulene. Two of the components, *E* β -caryophyllene and α -humulene were also evaluated using commercial caryophyllene samples. *Z*-Caryophyllene, present in the commercial sample was also evaluated. Two sets of hydrocarbon standards, n-alkanes and a series of relatively unrelated cyclic compounds that included adamantane and two alkyl derivatives, (-) α -pinene, diamantane and 1,4-di-*t*-butylbenzene, were used. Vaporization enthalpies of the targets at $T = 298.15$ K were reproduced within the specified uncertainties by both sets of standards as were vapor pressures from $T = (298.15$ to $\sim 400)$ K. Above 400 K, vapor pressures diverged. Equations for the evaluation of vapor pressure as a function of temperature are reported for all four compounds investigated

Keywords: *E* β -Caryophyllene; *trans* α -Bergamotene; *Z*-Caryophyllene; Vapor pressure; Vaporization Enthalpy; Correlation gas Chromatography

This article is dedicated to the contributions of Professor Gennady J. Kabo on the occasion of his 80th birthday.

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