PHYSICOCHEMICAL PROPERTIES AND VAPOR-LIQUID EQUILIBRIUM DATA FOR STEAM-DISTILLED LEMON ESSENTIAL OIL

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***Abstract*— Density and refractive index for steam-distilled lemon essential oil were obtained at several temperatures and vapor pressure measurements over the pressure and temperature ranges of P= (2.5 to 80.0) kPa and T = (342.57 to 440.39) K, respectively. Dependence with temperature for these experimental results were fitted to empirical polynomial relations, in order to obtain their coefficients and standard deviations. Calculated values are in good agreement with the experimental ones. The molar enthalpy of vaporization for steam-distilled lemon essential oil was calculated plotting the logarithm of the vapor pressure against the reciprocal temperature. Vapor-liquid equilibrium data of some key components were also obtained over the pressure and temperature ranges of P = (10.0 to 80.0) kPa and T = (374.46 to 440.39) K, respectively. Compositions of both equilibrium phases were determined for these key components by gas chromatography (GC). The essential oil components were characterized by their GC-retention times and the results are compared with gas chromatogram (GC/ MSD) data previously reported in the literature.**

***Keywords*— Steam-distilled lemon essential oil; Vapor-liquid equilibrium; Density; Refractive index; Vapor pressure.**

I. INTRODUCTION

Tucumán, located in northwest of Argentina, is an important producer of lemon essential oil (Sinclair, 1984). It is mainly obtained by using extractor machines (Bauer *et al.*, 2001; Dewick, 2002; Baser, 1995), which simultaneously extract oil and juice from the lemon fruit. Cold pressed lemon peel oil is a valuable raw material for food, cosmetic, and perfume industries because of its typical citrus flavor. The essential oil is a complex mixture constituted by more than a hundred compounds, such as monoterpenes (> 90 percent of the oil), monoterpene oxygenated derivatives (linalool, citral, esters, etc.), sesquiterpenes (C_{10} and C_{15} terpene unsaturated hydrocarbons) and a non-volatile residue constituted by waxes, pigments, coumarins, and psoralens (Braddock, 1999; Hui, 1992). The concentration of these components depends of several factors, such as the fruit variety, processing conditions, weather, soil, degree of maturity of the fruit, etc.

Cold pressed lemon essential oil is a yellow to yellow-greenish colored liquid with a natural fruit aroma characteristic of the lemon from which it is obtained. However, the steam-distilled essential oil is a colorless liquid, which has a similar aroma to the cold pressed oil but practically does not have any non-volatile residue. The lack of color of the steam-distilled essential oil, due to the absence of pigments and coumarins, is one of the most important differences with respect to the cold pressed essential oil, because it leads to very different ultraviolet absorption spectra (Sale, 1953).

Physicochemical properties such as density, refractive index, vapor pressure, and vapor-liquid equilibrium (VLE) data are useful for a full understanding of the thermodynamic properties, as well as for practical chemical engineering purposes.

In this paper we report density ρ and refractive index n_D at several temperatures, and vapor pressure P data over the pressure range P = (2.5 to 80.0) kPa for steam-distilled lemon essential oil (obtained from the EUREKA lemon variety). Vapor-liquid equilibrium data are also reported over the pressure range P = (10.0 to 80.0) kPa. From these last experimental results, we study how some key lemon oil components (α-thujene, α-pinene, sabinene, β-pinene, *d*-limonene, γ-terpinene, neral, and geranial) are fractionated between the liquid and vapor phases. These compounds are very important because they have a significant impact on the top notes of lemon essential oil.

Empiric equations for density, vapor pressure, and refractive index for the sodium D-line of the essential lemon oil as a function of the temperature were developed. These equations are useful for interpolation data within the studied temperature range. Furthermore, the molar enthalpy of vaporization was calculated from the dependence of the logarithm of the vapor pressure with the reciprocal of temperature. All empiric equations were fitted with polynomial equations, in order to obtain their coefficients and standard deviations.

Although the properties of the steam-distilled lemon essential oil could change slightly among different lots as a consequence of changes in the processing conditions, lemon variety, etc., these experimental values can be considered as representative of this lemon oil type. Furthermore, thermodynamic properties of natural products are rather rare in the literature and no experimental values for the studied essential oil could be found.