THERMODYNAMIC PROPERTIES OF MOLDY-MUSTY CONTAMINANTS OF WINE

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The wine industry is the main target sector of cork products through cork stoppers manufacturing. Despite the technical advantages of using cork stoppers to seal wine bottles, corks can transfer taint to wine due to the aroma-intense compounds present in the cork. This off-aroma, described as "moldy-musty," is commonly related to the chloroanisole family of compounds. 2,4,6-Trichloroanisole (TCA) is considered the most important contributor to the sensory deviations related to cork due to its particularly low sensory threshold [1]. Other musty-smelling compounds, such as 2,4,6-tribromoanisole (TBA), 2,4,6-tribromophenol (TBP) and 2,4,6-trichlorophenol (TCP), have also been identified as contributors to off-flavors in wines. In order to study the volatility of those compounds, it was decided to perform a thermodynamic study of phase transitions of TCA, TBA and TBP [2]. The vapor pressures of both crystalline and liquid phases of the three compounds were measured using a static method based on capacitance diaphragm manometers [3]. Moreover, the sublimation vapor pressures of TBP were also measured using a Knudsen mass-loss effusion technique [4]. The standard molar enthalpies, entropies, and Gibbs energies of sublimation and of vaporization, at reference temperatures, were derived from the experimental results as well as the (p,T) values of the triple point of each compound. The temperatures and molar enthalpies of fusion of the three benzene derivatives were determined using DSC. The thermodynamic results were discussed together with the available literature data for TCP [5,6]. To help rationalize the phase behavior of these substances, the crystallographic structure of TBP was determined by single crystal X-ray diffraction.

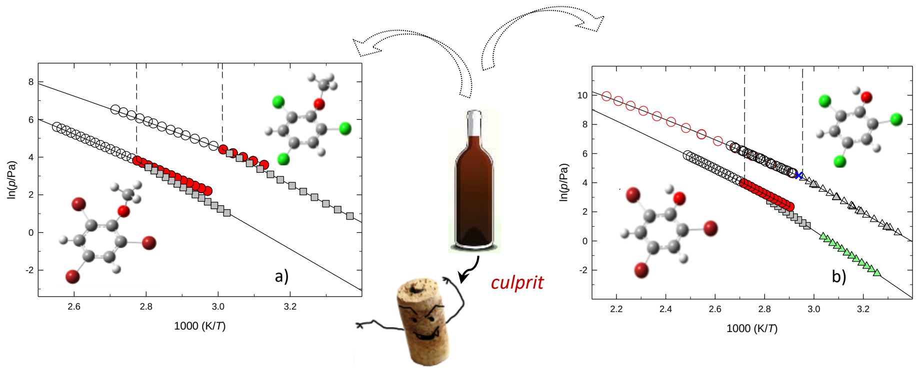

Fig.1. a) **Phase diagrams of TCA and TBA**. ○, vaporization; ●, vaporization (supercooled liquid); ■, sublimation (static method). b) **Phase diagram of TBP and TCP**. TBP: ○, vaporization; ●, vaporization (supercooled liquid); ■, sublimation (static method); ▲, sublimation (Knudsen effusion method); TCP: ○, vaporization (transpiration method [5]); ○, vaporization (static method [6]); Δ, sublimation (transpiration method [5]); ▲, sublimation (static method [6]); ×, result related to sublimation according to [5].

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