THERMOCHEMICAL FINGERPRINT OF ALLYL CINNAMATE

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The main disposal pathway of the highly-fragranced consumer goods we use every day is the urban wastewaters. The environmental monitoring carried out over the past 20 years has verified that most of the fragrance compounds are not removed with conventional wastewater treatment technologies. The continued release of these chemicals with wastewater effluent will cause long-term hazards due to its persistence and ability to bioaccumulate, with unknown consequences for aquatic life and the food chain. Recently, the scientific community has recognized fragrances as emerging pollutants in aquatic systems [1,2].

The objective of this work is to evaluate and discuss the energetic properties of the chemical fragrance allyl cinnamate (figure 1), through experimental and computational studies in order to provide reliable data for its environmental risk assessment.

Static-bomb combustion calorimetry and Calvet microcalorimetry techniques were used to get the enthalpy of formation in the liquid phase and the enthalpy of vaporization, respectively, of the compound under study. In turn, this data enabled to derive the gas-phase standard molar enthalpy of formation of this compound, at T=298.15 K. Theoretical studies, using the G3(MP2)//B3LYP composite computational method, were also performed to obtain the same gas-phase thermochemical parameter.

Structural changes and the inherent energetic effects are analysed and compared with those for ethyl (*E*)-cinnamate [3].

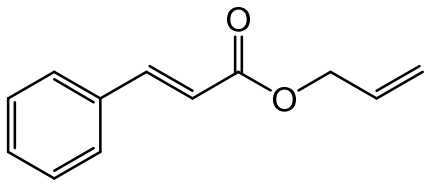

Figure 1. Structural formula for allyl cinnamate
(IUPAC name: prop-2-enyl (*E*)-3-phenylprop-2-enoate).

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[3] C A. O. Silva, V. L. S. Freitas, M. D. M. C. Ribeiro da Silva (2021, January 27-28). Thermochemical study of cinnamate derivatives [Conference presentation abstract], XLII National Conference on Calorimetry, Thermal Analysis and Applied Thermodynamics, Udine, Italy.