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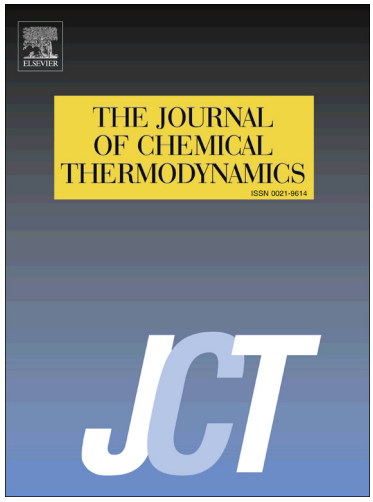

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Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

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Abstract

In this work, we present experimental and theoretical thermochemistry of the 3- and 4-nitrophtalic acids. We report their standard molar enthalpies of formation in crystalline phase, at T = 298.15 K, which were obtained from their energies of combustion. The latter were determined through an isoperibolic bomb calorimeter. We measured the change-phase enthalpies, as well as the fusion and sublimation enthalpies, by differential scanning calorimetry (DSC) and thermogravimetry (TG). Also *via* DSC, we found the heat capacity equations (in crystalline phase) for both isomers as functions of temperature. We determined the enthalpies of formation in both crystal- and gas-phase from the previous measurements. In addition, we computed the enthalpies of formation in gas-phase of both isomers using the composite Gaussian-G4 method and atomization reactions. The final theoretical enthalpies were computed using a weighted Boltzmann averaging procedure, and the weights were estimated using the Gibbs free energy at T = 298.15 K. The absolute differences between theoretical and experimental enthalpies are below 3.3 kJ·mol^{-1}. Finally, we apply our results for obtaining the isomerization enthalpy of 3- to 4-nitrophtalic acid, and difference enthalpies between the nitrophtalic acids and their anhydrides.

Keywords: 3- and 4-nitrophthalic acids, combustion, formation enthalpy, theoretical study.

1. Introduction

3- and 4- Nitrophthalic acids are commonly used in the production chains of a wide variety of commercial products such as pigments, dyes, plasticizers, *etc.* [1]. They are also used as precursors of 4- and 5-nitro-2-benzofuran-1,3-dione, which in turn are used as intermediate reactants in polypeptide synthesis [2]. The nitrophthalic acids constitute

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