Calorimetric and computational study of methyl 1*H*-1,2,4-triazole-3-carboxylate

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Substituted triazoles can present biological activity and they are used in pharmacology due to their anti-inflammatory and anti-viral properties. As examples, it is possible to refer the methyl 1*H*-1,2,4-triazole-3-carboxylate derivatives as anti-inflammatory agents in pathological disorders, namely the atherosclerosis and rheumatoid arthritis. [1,2] In addition, the title compound has been used as a starting material for ribavirin (1-D-ribofuranosyl-1,2,4-triazole-3-carboxamide), a nucleoside analogue that has demonstrated efficacy in treating respiratory syncytial virus infection, hepatitis C and some viral hemorrhagic fevers. [3]

The thermodynamic characterization of this type of compounds may be relevant for the understanding of their reactivity. In this context, the present work reports a calorimetric and computational study of methyl 1*H*-1,2,4-triazole-3-carboxylate (Figure 1). The enthalpies of combustion and sublimation of this compound were determined from static bomb calorimetry and Calvet microcalorimetry, respectively. From these data, the corresponding gas phase standard molar enthalpy of formation was derived. Additionally, the gas phase standard molar enthalpy of formation was obtained from high level *ab initio* calculations, at the G3(MP2)//B3LYP level of theory.[4] The computational approach also allowed to establish the molecular structure, taking into consideration the different stable conformations.

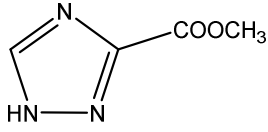

Figure 1 − Molecular structure of methyl 1*H*-1,2,4-triazole-3-carboxylate

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