AN OVERVIEW OF ENERGETIC AND STRUCTURAL STUDIES ON KEY ORGANIC COMPOUNDS

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The study of thermochemical properties of key organic molecules as well as inherent relationships with structural characteristics is relevant on the establishment of predictive schemes for the energetic characterization of related species. Computational approaches are also being used in order to support the development of strategies allowing the establishment of the reliable prediction schemes. In addition, the evaluation of the corresponding thermodynamic stability of compounds is one of the main topics of our research group.

In this context, we have been involved in a systematic experimental and computational energetic study on selected organic compounds [1-3], namely 1,3-benzazoles, thiadiazoles and several other value-added chemicals derived from biomass.

The experimental data are essentially derived from calorimetric measurements, aiming to obtain standard molar enthalpies of formation in the condensed and gaseous phases. Some effusion studies are also performed to evaluate study phase transitions and to infer about the organization of the molecules in the condensed phase.

It is noteworthy that the thermodynamic properties allow a rigorous interpretation of the chemical and/or physical transformations in which the compounds are involved, considering their use in innumerous applications in different fields, in particular in chemical industries.

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