Assessing the self-polymerization hazards of substances by theoretical chemistry

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ABSTRACT

Polymerizing substances are substances which, without stabilization, are likely to undergo a strongly exothermic reaction leading to the formation of larger molecules or polymers under specific conditions like transport. Their uncontrolled polymerizations are implicated in industrial accidents, particularly incidents of polymerization runaway during chemical industrial processes or transport in tankers.

For these reasons, a specific classification for these substances was introduced in 2013 in the Recommendations on the Transport of Dangerous Goods (TDG)[1]. They are classified based on criteria primarily developed for self-reactive substances and organic peroxides. However, their unique reactivity mechanisms may necessitate testing and adaptation of classification criteria.

In this context, understanding reaction mechanisms is crucial for identifying polymerizing substances and accurately distinguishing between self-reactive and polymerizing substances, prompting exploration into theoretical studies using DFT quantum chemical methods to complement experimental testing.

Based on a first theoretical study of the self-polymerization of styrene and derivatives, this study aims to extend this analysis to other kind of polymerizing substances and define theoretical chemistry approaches to help classify these hazardous substances and favor their safe transport and use[2].

References

[1] UN Recommendations on the Transport of Dangerous Goods - Model Regulations, Reference Manual ST/SG/AC.10/1/Rev.21, **2019**

[2] Fayet G., Rotureau P., Vicot P. On the hazard investigation of polymerizing substances through experimental methods and theoretical chemistry. *Chemical Engineering Transactions*, **2022**, *90*, 367-372.