

Density Functional Theory Study of 1,3-dipolar cycloaddition and Solvent Effects

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Abstract

The 1,3-dipolar cycloaddition reaction is the main method to obtain heterocyclic compounds in good yields. Huisgen reaction using nitrene and olefins containing active double bonds such as maleimide, is widely used to synthesise five-membered heterocyclic derivatives like isoxazolidine. However, the current trend of organic synthesis is the use of green chemistry, and ecofriendly processes. In this fact, recently, Bhaskar Chakraborty and Prawin K. Sharma reported a diastereo and regioselective synthesis of some novel isoxazolidine derivatives by one pot cycloaddition reactions between nitrene and different maleimides in aqueous phase. The result has shown that form *exo* is more dominant. The results of the energy ΔE_r , the enthalpy ΔH_r and the free enthalpy ΔG_r of the reaction, the activation energy ΔE^\ddagger , the enthalpy of activation ΔH^\ddagger and the free activation enthalpy ΔG^\ddagger at 298.15 K in the aqueous solution have shown that *exo* product is more favoured kinetically and thermodynamically than the *endo* product. For the kinetic solvent effects of this reaction, among the four solvents used, water was found to be the best and the most convenient medium for the course of this reaction.

Speaker Publications:

1. "Microwave-assisted synthesis of new imide-and formamide-derivatives of 2(3H)-benzoxazolinones and 2(3H)-benzothiazolinones ; Archive for organic chemistry; vol 04, 2017, 315-329.
2. "Experimental and theoretical investigation of the intramolecular cyclisation of N-(benzoxazolinon-6-YI) Maleimide derivatives"; 2015.
3. "Synthesis of some novel benzoxazolinonylcarboxamides as potential anti-inflammatory agents"; Journal of Chemical Research; vol 38, 204.
4. "Rapport de Mission de Suivi et de Restructuration du Projet d'Aménagement du Parc d'El Kala et du Complexe de Zones Humides"; 1998.

[6th International Conference on Physical and Theoretical Chemistry](#); Webinar; March 18 -19, 2020.

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Biography:

Seddiki Khemissi is currently working as faculty member at Laboratory of Synthesis and Organic Biocatalysis (LSBO), Faculty of Sciences of the University BADJI Mokhtar – Annaba in Algeria. He attended many conferences and published his work in reputed journals.