

Investigation of the regioselectivity of thermal cyclization reactions in gas and liquid phase high temperature flow reactors

Richard Jones, Gellert Sipos, Laszlo Lengyel, Gyorgy Dorman, Laszlo Kcosis, Heather Graehl, Ferenc Darvas

Thalesnano, Budapest, Hungary

Gould-Jacobs type intramolecular thermal cyclisations were previously reported in a continuous flow reactor at high temperatures (300-360C) and pressure (100-160bar) in liquid phase. The regioselectivity of the ring closure depends on the nature and position of the substituents often leading to a mixture of products. We investigated the regiochemical outcome of substituted amino-pyridine substructures cyclisation under various conditions in liquid and gas phase as well, applying a flow pyrolysis apparatus under high vacuum between solvent-free conditions. Flash vacuum pyrolysis (FVP) allows a rapid exposure to high temperature (200 – 900C), which often favour the formation of one regioisomer. Here we compare the outcome of the thermal cyclisation of various unsaturated diesters or analogue substructures (derived from condensation with ethoxymethylenomalonate) performed in both systems.

