Title: Polymerization with phosphonium-organocatalysts: A kinetic study

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The kinetic study results of acrylonitrile (AcN) polymerization with phosphonium-organocatalysts are presented herein. The influence of temperature, steric hindrance, base ratio, activation time and phosphonium dilution has been qualitatively determined. A detailed quantitative study of the temperature dependence has been carried out, showing this polymerization to be a 0 order reaction, with a rate constant value of k=4.1717 mol·dm-3·min-1 at -30 °C (as the highest constant rate), obeying the Arrhenius equation and with an activation energy value of Ea= -9.028 kJ·mol-1. Best conditions for the fastest polymerization of AcN are found out to be: -30 °C, Trimethylphosphonium tetrafluoroborate as phosphonium salt, potassium carbonate as base, 100 base to phosphonium ratio, 10 min activation time and a low phosphonium dilution factor. Number average molecular weights (Mn) and polydispersity index (PDI) values have been obtained by GPC measurements and kinetics have been followed with ¹H-NMR measurements: in order to plot the yield as a concentration dependent measurement.

Keywords: Anionic polymerization, acrylonitrile, phosphonium, catalysis, kinetic.

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