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mgr inż. Magdalena Litwinowicz

„Studies on the carbamate esters synthesis reactions”

Promotor: prof. dr hab. inż. Jacek Kijeński, Prof. dr hab. inż. Jacek Kijeński
Instytut Chemii Przemysłowej w Warszawie
Politechnika Warszawska Filia Płock
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The purpose of the work was to study the reaction of organic carbamate esters synthesis by reaction of amines with dimethyl carbonate. It is an environmentally friendly alternative to the phosgene technology used in the traditional synthesis of carbamates. Carbamate esters are compounds widely used in the pharmaceutical industry (anticancer and antiviral drugs), agricultural industry (plant protection products), polymer industry (the production of foams, coatings, binders and plastics) as well as in organic synthesis (protective groups).

In order to achieve the aim of the work, a number of carbamate esters were synthesized using different amines and different reaction conditions. The work was divided into 5 research parts:

The reactions carried out in a batch system were first investigated. The influence of process parameters such as temperature, pressure and reaction time on the reactivity of selected amines was examined. The influence of structure and order of amines on their reactivity in reaction with dimethyl carbonate was demonstrated.

Based on the results obtained in the first part of the work the kinetics of the amine methoxycarbonylation reaction was investigated by determining the amine concentration change during the reaction. The kinetic equations for individual reactions were defined, the orders of reactions were determined, the values of observed reaction rate constants and the half-life times were calculated. The activation energy of the N-hexylcarbamate synthesis reaction was also calculated and the mechanism for the reaction of methoxycarbonylation of the amines with dimethyl carbonate was proposed.

The third part of the work involved reactions of carbamate esters synthesis in a continuous system. A reaction set-up was designed and the influence of basic parameters on the obtained results was examined. It was the first time that the reaction of methoxycarbonylation of the amines with dimethyl carbonate was carried out in a continuous system.

The next part concerned the use of heterogeneous catalysis in the synthesis of carbamates by described method. The activity of six heterogeneous catalysts was tested in a continuous system.

Additionally, based on literature reports, a series of reactions were carried out with the participation of supercritical carbon dioxide, both in a batch and in a continuous system. No positive effect of CO₂ was observed.

All research results and conclusions presented in my work significantly deepen the knowledge about methoxycarbonylation reaction and go beyond the state of knowledge contained in the literature.

Magdalena Litwinowicz
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