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Doctoral Dissertation

Badania nad katalityczną racemizacją w dynamicznym rozdziale kinetycznym

Investigations on catalytic racemization in dynamic kinetic resolution

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Abstract

Dynamic kinetic resolution (DKR) is a complex process dedicated to secondary alcohols and primary amines, leading to obtaining enantiomers with high yields. In this process the cooperation of two catalysts is very crucial. Commonly used catalysts are: a metal complex compound as a racemization catalyst and an enzyme for enantionselective synthesis. The main group of metal catalysts with racemization properties are ruthenium complexes.

In the presented doctoral dissertation, the first part is a literature study on the DKR process with particular emphasis on the catalysts used in it. Racemization process also has been widely described.

The following part of the work describes the method of preparation, characterization and racemization properties of selected ruthenium complex compounds. Moreover, the work discusses the topic of immobilization of ruthenium compounds on silica and carbon supports, leading to the preparation of heterogeneous racemization catalysts. In this doctoral thesis, not only the synthesis of catalysts is very important, but above all the analysis of their racemization properties and the possibility of using them in DKR. The catalytic activity of the obtained compounds was determined in the racemization reaction of the secondary alcohol (*S*)- 1-phenylethanol and (*S*)-1-(1-naphthyl)ethanol. The DKR process was carried out using the most active racemization catalysts. As part of this work, the effect of the addition of ionic liquid on the rate of the racemization process involving ruthenium complexes was also investigated and described. The research carried out and the information obtained from it led to the design and creation of a heterogeneous system in which the main components are: a ruthenium complex, an ionic liquid, an activating base, an enzyme and a small amount of solvent. The formation and subsequent separation of two phases allowed both the enzyme and the ruthenium complex to be used several times in the DKR process.

The research carried out and its results were described in three publications from the JCR list and became the subject of one national patent and eight conference presentations.