The Calculation for Optimized Structure of Enantioselective Catalyst in Arylation of α-Imino Ester

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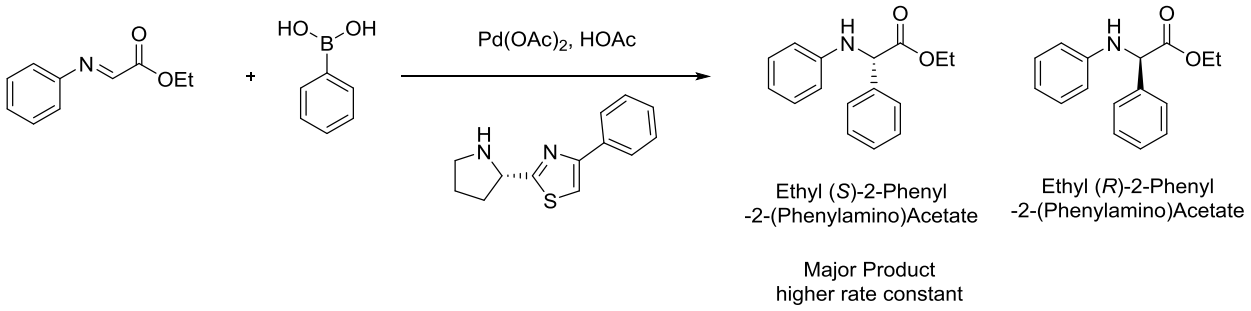
Abstract: The arylation of alpha-imino ester is one of important reactions for synthesis of amino acid derivatives that can be used as precursor for synthesis of several bioactive compounds. Computational chemistry is a powerful tool to predict the product of the reaction, especially, the reaction giving enantiomer products. In this research work, asymmetric synthesis reaction using Ethyl (E)-2-(Phenylimino)Acetate and Phenylboronic Acid as precursor, Palladium(II)Acetateas catalyst, and (S)-4-Phenyl-2(Pyrrolidin-2-yl)Thiazoleas ligand, was calculated. The B3LYP method, which belongs to Density Functional Theory,was selected. The cc-pvdz basis set was used for all atoms except palladium atom in which the LANLDZ basis set was used for Electronic Core Potential. The results show that Ethyl (S)-2-Phenyl-2-(Phenylamino)Acetate is more preferable as a product than Ethyl (R)-2-Phenyl-2-(Phenylamino)Acetate because of the kinetic control factor, in which it has higher rate constant.



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