

Mechanistic Studies of the Organocatalyzed Diels-Alder Reaction Through Linear Free Energy Relationships

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Palavras Chave: Diels-Alder reaction, Organocatalysis, LFER, (E)-chalcone.

Highlights

Linear Free Energy Relationships of the Diels-Alder reaction between cinnamaldehydes and dienes via aminocatalysis.

Resumo/Abstract

This work aims to investigate the influence of substrate electronics in organocatalyzed Diels-Alder reactions between α,β -unsaturated aldehydes (cinnamaldehydes) bearing a *p*-substituted aryl groups and a dienes bearing two more. The dienes of these studies were prepared from Wittig olefinations of chalcones, which were themselves prepared from aldolic condensations of *p*-substituted acetophenones and *p*-substituted benzaldehydes. For this study, both electron donating and electron withdrawing groups were used in order to obtain insights of their influence in the reactivity and selectivity through Linear Free Energy Relationships (LFER). A comparison between Jørgensen-Hayashi and MacMillan' organocatalysts was also performed.

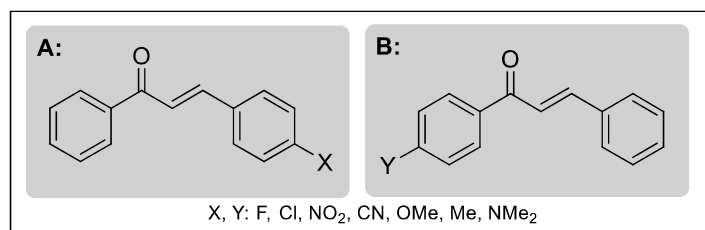


Figure 1. (E)-chalcones obtained from substituted benzaldehydes (A) or substituted acetophenones (B).

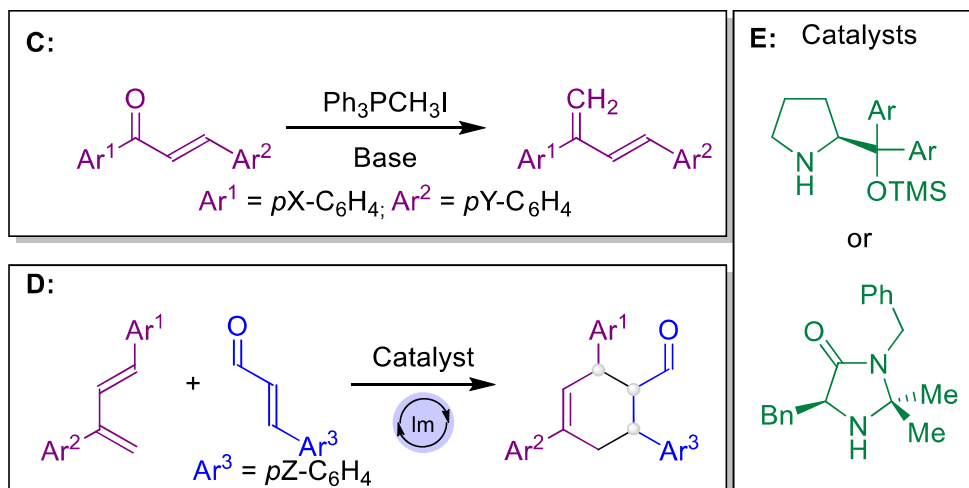


Figure 2. C: Wittig reaction scheme in order to obtain the conjugated diene. D: Diels-Alder reaction for LFER. E: Catalysts

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