

# Mechanistic Investigations on the Benzylation of $\beta$ -Ketoesters via Cooperative Catalysis

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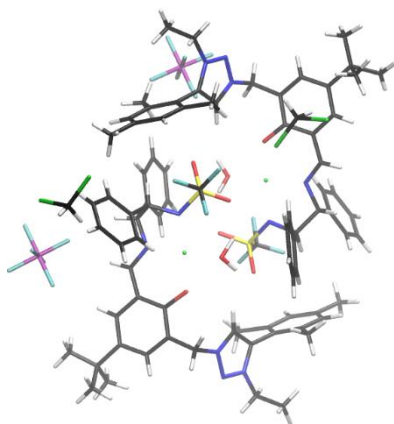
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## Abstract:

One of the main synthetic challenges is the reliable and industrially achievable formation of carbon-carbon bonds. One important reaction type to form such bonds are benzylation reactions, where a benzyl moiety is introduced using a nucleophilic carbon species. In most cases this leads to tertiary carbons, likely forming stereocenters, which makes these types of reactions highly interesting for catalysis and stereoselective control. We present the benzylation of  $\beta$ -ketoesters via asymmetric cooperative catalysis using copper-based catalysts. Previous work showed promising results for this type of reaction [1]. We present results for the benzylation of  $\beta$ -ketoesters using benzylbromide as a benzylation agent producing high yields and selectivities of up to 94 %e.e. On this poster mechanistic investigations using computational chemistry methods are highlighted giving further insight into rate-determining steps and stereo-control of the reaction. With these insights further catalyst designs are possible.



[1] A. C. Hans, Andreas C., *et al.* Angew. Chem., Int. Ed., **2023**, 135, e202217519