DoE-Assisted Development of a 2H-MoS_2-Catalyzed Approach for the Production of Indole Derivatives

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2H-MoS_2 is an appealing semiconductor material due to its earth-abundant nature, cheapness, and low toxicity.[1] Although 2H-MoS_2 has shown promising catalytic activity for various energy-related processes, its use in the catalysis of C-C bond forming reactions is still largely unexplored. The lack of examples in organic synthesis is mostly a consequence of the intrinsic difficulties of using bulk 2H-MoS_2 (*e.g.*, low surface area), which implies the use of high catalytic loadings.[2] In our research, we have focused on the development of a 2H-MoS_2-mediated synthesis of valuable bisindolylmethane derivatives (**3**), using indoles (**1**) and benzaldehydes (**2**) as starting materials. Notably, with the aid of Design of Experiments (DoE) method, we have effectively established the optimal reaction conditions while also identifying the critical parameters affecting the catalytic performance of commercial 2H-MoS_2 powder (**Fig. 1**). Lastly, we have demonstrated that the catalytic system has large versatility and good tolerance towards functional group variations of the reagents.

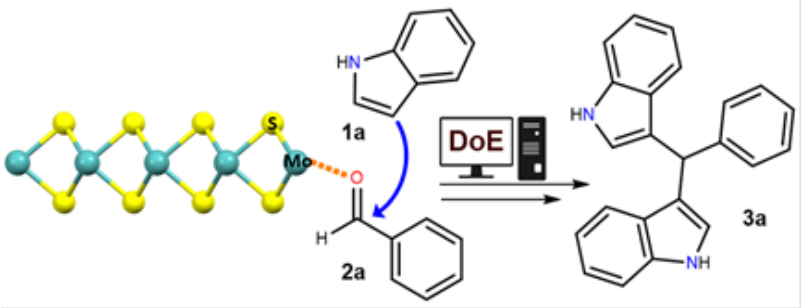

Figure 1. Schematic representation of the reaction between **1a** and **2a** to give **3a** catalysed by bulk 2H-MoS_2. For simplicity, bulk MoS_2 has been represented as a single layer.

References

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