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

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Transition metal dichalcogenides (TMDCs) represent a large family of solid compounds with unique electrical, mechanical, and optical properties.[1] Within this group of materials, 2H-MoS_2 is an appealing semiconductor material due to its earth-abundant nature, cheapness, and low toxicity.[2] 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 to yield useful organic compounds 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 for obtaining acceptable yields.[3] This aspect renders the overall optimization process more expensive, difficult, and tedious. In our research, we have focused on the development of a 2H-MoS_2-mediated synthesis of valuable bisindolylmethane (BIM) derivatives (**3**),[4] 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 (Figure 1).[5] Lastly, we have demonstrated that the catalytic system has large versatility and good tolerance towards functional group variations of the reagents. M. Morant thanks Margarita Salas grant (MS21-041) from the Universitat de València

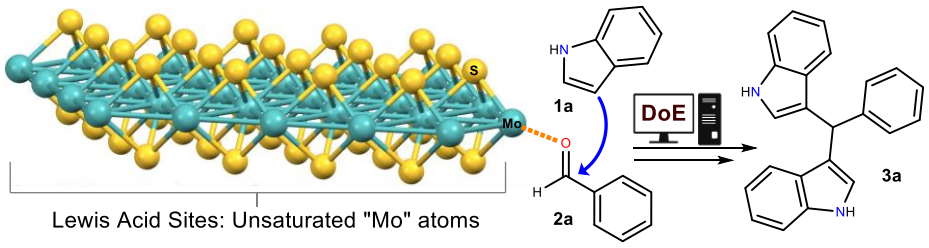

Figure 1: Schematic representation of the reaction between 1a and 2a to give 3a catalysed by bulk 2H-MoS_2.

References

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