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Title:	Mechanistic insight into the azo radical-promoted dehydrogenation of heteroarene towards N-heterocycles
Authors:	Bains, A.K. (/jspui/browse?type=author&value=Bains%2C+A.K.) Adhikari, D. (/jspui/browse?type=author&value=Adhikari%2C+D.)
Keywords:	hydrogenation-promoted annulations N-heterocycles. dehydrogenation
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Citation:	Catalysis Science and Technology, 10(18) pp. 6309-6318.
Abstract:	Borrowing hydrogenation-promoted annulations are considered to be important reactions to synthesize wide variety of N-heterocycles. In these processes, the dehydrogenation of saturated heteroarenes in the late stage is generally required to furnish the desired N-heterocycle. However, in a one-pot, multistep heterocycle synthesis, this step is not well elucidated, and the role of the catalyst is not thoroughly understood. Furthermore, the use of copious amount of base at elevated temperatures further complicates this matter and casts doubt on the involvement of the catalyst in heteroarene dehydrogenation. Herein, we report a molecularly defined nickel catalyst, which can perform two annulation reactions under mild conditions (80 °C, 8 h), towards the sustainable synthesis of triazine and pyrimidine. Mechanistically, we clearly describe the important role of the catalyst in promoting the dehydrogenation of heteroarenes. The binding of the saturated heterocycle to the metal catalyst undergoes a pre-equilibrium step ($K = 238$ at 80 °C), which is followed by a crucial hydrogen atom transfer. A series of kinetics experiments including Van't Hoff, Eyring analysis and interception of pyrimidinyl radical disclosed the details of the dehydrogenation process. This ligand-driven, base metal catalytic approach is significantly different from the considerably evaluated metal-ligand cooperative bond activation strategies, which may offer an alternative dehydrogenation pathway that demands less energy.
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