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Studying Deactivation phenomena using Pd/1,2-DTBPMB in the Tandem Isomerization- Methoxycarbonylation Reaction

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Homogenous palladium catalysts are widely used for the methoxycarbonylation of unsaturated compounds. However, catalyst deactivation primarily through the formation of Palladium black and ligand degradation, remains a key limitation for practical application. We report a systematic study to find optimal reaction conditions for a stable catalytic system which was scaled-up to study the recyclability. The catalyst was successfully recycled at larger scale without loss of catalytic activity or selectivity with no observable Pd black. Consequently, to determine the minimum effective catalyst loading, the catalyst concentration was further reduced, it could be recycled for up to four consecutive runs, a decrease in reactivity was observed in the fifth run. This loss in activity was attributed to extensive ligand oxidation, as confirmed by NMR spectroscopy. Based on these findings, the optimized catalytic system was subsequently scaled up, achieving sustained catalytic performance over six consecutive recycling cycles with a total turnover number (TON) of 10342.