Reductive N-methylation of amines using dimethyl carbonate and molecular hydrogen: mechanistic insights through kinetic modelling

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Reductive N-methylation of amines using dimethyl carbonate and molecular hydrogen: mechanistic insights through kinetic modelling

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Abstract

Kinetic analysis of ruthenium-catalyzed reductive N-methylation of amines using dimethyl carbonate as C1 source and molecular hydrogen has been performed. Kinetic equations have been derived and kinetic modelling has been performed for experimental data generated previously at a constant hydrogen pressure as well as for additional experiments performed at different hydrogen pressures. The study has revealed interesting kinetic features related to an induction period strongly influenced by temperature. A kinetic model has been proposed based on advanced reaction mechanism featuring transformation between different type of catalytic species and inactivation of them during the reaction. Kinetic modelling was done for all data sets together showing excellent correspondence between calculations and experiments.