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petro- and oleochemicals in
complex hydroformylation
reaction networks**



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The homogeneously rhodium-BiPhePhos catalyzed hydroformylation of renewable long-chain fatty acid methyl esters (FAME's) to polymer precursors is an important and promising example reaction for industrially relevant "Green Chemistry". A typical FAME of interest with internal double bond is methyl oleate, which can be produced from e.g. rapeseed oil. However, corresponding mechanistic kinetic models, needed for model-based process design and optimization, are still not available in the literature. Hydroformylation of substrates with internal double bond requires simultaneous double bond isomerization to produce linear aldehydes. If these substrates are esters, the ester group could in principle interact with the hydroformylation catalyst and affect its activity. These issues have to be understood in order to be quantified by mechanistic kinetic models. Hence, two model compounds were used in this thesis to study the kinetics of double bond isomerization, hydrogenation and (tandem isomerization-) hydroformylation reactions with and without ester-catalyst interactions: 1-decene as typical long-chain olefin and the structurally analogous and renewable FAME methyl 10-undecenoate. The reaction mechanisms of both substrates were investigated using operando ATR-FTIR spectroscopy to observe catalyst resting states and derive rate determining steps.