

Halogenated rhodium(I) complexes as model catalysts for methanol carbonylation

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Catalysis plays a vital role in numerous stages of petroleum refinement and fuel production, with one of the major energy sources globally being crude oil for fuels and further production of a variety of chemicals [1]. However, development of highly selective catalysts still poses a significant challenge in many of these processes [2]. Methanol carbonylation is one of the major homogeneously catalysed process for production of the acetic acid from methanol. With the oxidative addition of methyl iodide being the rate determining step in this catalytic process; the selectivity of the catalyst to favour the formation of the desired product may be achieved by carefully varying the ligand system of said catalyst as well as the reaction conditions [3].

The selectivity for acetic acid production with rhodium-based catalysts in a homogeneous medium is roughly

99% [4]. Catalytic rhodium system's activity and selectivity are vastly improved by phosphine ligands leading to favourable results under milder conditions [5].

Our functionalised halogenated rhodium(I) complexes, $[\text{Rh}(\text{N},\text{O})(\text{CO})(\text{PR}_3)]$ ($\text{R} = \text{Ph}, \text{Cy}$), coordinated to N,O bidentate Schiff-base ligands and select phosphine ligands are hereby reported. The extensive structural characterization of the complexes followed by the kinetic mechanistic study using UV/Vis, infrared and nuclear magnetic resonance spectroscopy will also be reported. The influence of halogens (F, Cl, Br) on the para-position of the Schiff base ligand on the methyl iodide oxidative addition to the rhodium(I) monocarbonyl specie will also be described.

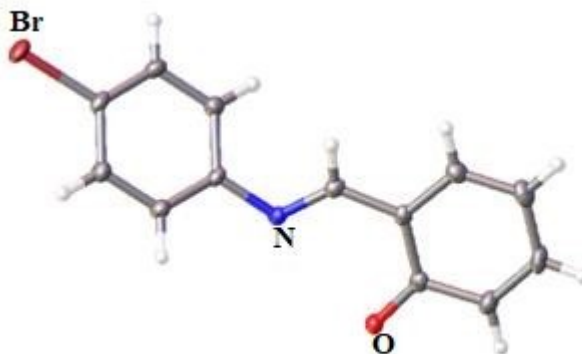


Figure 1: The crystal structure of the functionalized N-(4-bromido)-salicylaldehyde ligand system under investigation during the carbonylation of methanol. .

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