

## Molecular interactions in Supported Ionic Liquid Phase (SILP) catalysts for hydroformylation: A combined in situ IRAS and DFT study

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In supported ionic liquid phase (SILP) systems, an ionic liquid (IL) phase immobilizes a catalytically active metal complex, thus combining the advantages of homogeneous and heterogeneous catalysts. A prominent application of SILP systems is hydroformylation, e.g. over Rh-based systems. Recently, we showed that the IL and CO (ligands) suppress the formation of NPs from the molecular Rh complex.[1] In this work, we systematically investigate molecular interactions in custom-made SILP wafers based on [Rh(acac)(CO)<sub>2</sub>], xantphos, [C<sub>4</sub>C<sub>1</sub>Im][NTf<sub>2</sub>] and SiO<sub>2</sub> via IR spectroscopy in transmission (TIRS) and reflection absorption (IRAS) mode. With the help density functional theory (DFT) calculations, we identify the Rh complexes as a function of the composition of the SILP and the reaction conditions. Our results provide insights into an extended network of Rh species (including mixed [NTf<sub>2</sub>]<sup>-</sup> / xantphos / acac hydride and carbonyl complexes) which can be interconverted dynamically. The extension of the spectroscopic studies of SILP systems to (PM-)IRAS opens exciting possibilities for further studies.

[1] E. Kratzer *et al.*, *Catal. Sci. Technol.*, **2023**, 13, 2053–2069, 10.1039/D2CY02058K.