

Poster Presentations

[MS25-P21] Stereochemistry of Disordered Fluorinated Precursors of NHC

Ligands.

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NHC's (nitrogen heterocyclic carbenes) recently emerged as powerful ligands for transition metal complexes. For example, they are a part of ruthenium-based 2nd generation Grubbs and Hoveyda-Grubbs complexes, highly efficient catalysts for alkene metathesis.[1] Introduction of polyfluorinated alkyl chains into the molecule is a promising way to recycle the catalyst utilizing special fluorous separation techniques.[2] While compounds with less than 40 % of fluorine can be recycled by light fluorous techniques as fluorous solid phase extraction (FSPE), heavy fluorous techniques require the content of fluorine higher than 60 % and utilise different solubility in organic and perfluorinated solvents. As the key precursors of fluorous NHC ligands, we synthesised several variants of polyfluoroalkylated vicinal diamines. New intermediates of NHC ligands were studied by several analytical methods. Due to the nature of the polyfluorinated alkyl chains, the formation of single-crystals is a rare event, usually accompanied with heavy disorders. Moreover, the highly fluorophilic chains tend to self-assembly to create layers, which probably amplify the effect of the chains disorder. The reaction pathway, comparison of X-ray single-crystal structures of new NHC ligands and calculated models will be presented.

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[1] Vougioukalakis, G.C., Grubbs, R.H. (2010), *Chem. Rev.* 110 1746-1787.

[2] J.A. Gladysz, D.P. Curran, I.T. Horváth, Eds., *Handbook of Fluorous Chemistry*, Wiley-VCH, Weinberg, 2004.

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