FIRST PREPARATION OF IRIDIUM-N-XantPhos IMMOBILIZED CATALYSTS FOR QUINOLINE HYDROGENATION

Ivanytsya M. O.[1,3,4], Subotin V. V.[1,3], Mischenko A. M.[1], Tarasova I. V.[1], Velbovets A. R.[4], Ryabukhin S. V.[1,4], Volochnyuk D. M.[1,2,4], Kolotilov S. V.[3]

[1]Enamine Ltd, Kyiv, Ukraine

[2]Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine

[3]L.V. Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Kyiv, Ukraine

[4]National Taras Shevchenko University of Kyiv, Kyiv, Ukraine

ivanytsya.mykyta@gmail.com

Hydrogenation of organic heterocycles is an important process of a modern fine organic and medicinal chemistry, and organometallic phosphine-containing complexes of iridium are efficient homogenous catalysts for such transformation [1]. However, the use of such systems is associated with complicated purification of the products and significant losses of precious metals. Anchoring catalytically active metal coordination compounds on solid supports allows to combine the advantages of both homogenous and heterogenous catalysis. The creation of immobilized catalysts with high activity and stability during repeated use is still a challenging task [2].

Our goal was to obtain a hydrogenation catalyst suitable for repeated use on the basis of Iridium-N-XantPhos complex anchored to the SiO_2 surface. N-XantPhos was chosen due to its commercial affordability and ease of further modification *via* backbone N-H bond. $Si(OEt)_3$-modified N-XantPhos ligand (compound **2**) was synthesized and consequently two iridium-containing composites (**B1** and **B2**) were obtained by varying order of complexation and anchoring (Fig. 1a). Both composites were tested in the hydrogenation of quinoline under two sets of conditions (Fig. 1b) and the possibility of catalyst recycling has also been checked. It was found that usage of both composites in quinoline hydrogenation leads to a quantitative yield of tetrahydroquinoline at 100ºC and 100 atm of hydrogen. However, only composite **B2** retained high efficiency after the second run.

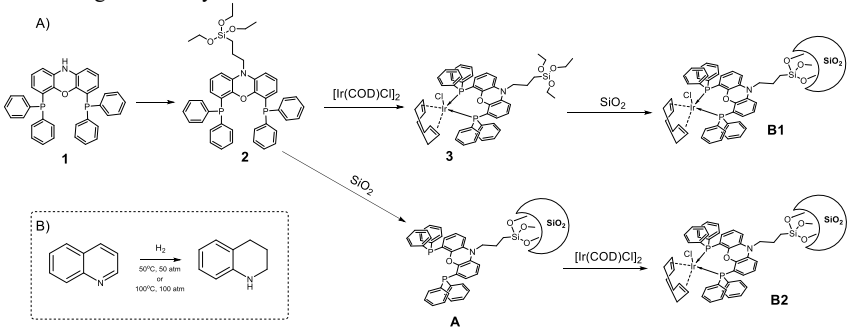

Fig. 1. a) synthetic route for **B1** and **B2** Ir-containing composites; b) hydrogenation of quinoline reaction

1. M. G. Manas, L. S. Sharninghausen, E. Lin, R. H. Crabtree. *Journal of Organometallic Chemistry*, **2015**, 792: 184–189

2. M. O. Ivanytsya, S. V. Ryabukhin, D. M. Volochnyuk, S. V. Kolotilov. *Theoretical and Experimental Chemistry*, **2020**, 56: 283–308