Abstract

The presented master thesis is devoted to the investigation of reaction intermediates in homogeneous gold catalysis. Electrospray ionization mass spectrometry (ESI-MS) was used as the primary research technique in this study. Delayed reactant labeling was used as the main method. I have focused mainly on the hydration of 1-phenyl-1-propyne catalyzed by the gold complex $[Au(IPr)(MeCN)]BF_4$ (IPr = 1,3-bis(2,6-di-iso-propylphenyl)imidazol-2-ylidene).

I have detected two main intermediates containing one or two gold atoms, respectively (monoaurated and diaurated intermediate). I have obtained rate constants for the degradation of the reaction intermediates and their half-lives. I have derived kinetic isotope effects for the formation and the decomposition of the detected intermediates. I have shown that the kinetics of the degradation of both intermediates is identical, therefore I conclude that hydration of alkynes catalyzed by gold complex [Au(IPr)(MeCN)]BF₄ proceeds most probably via neutral monoaurated intermediates. These neutral intermediates are detected by ESI-MS as protonated (monoaurated intermediate) or tagged by a second gold cation (diaurated intermediate).

Key words: gold catalysis, reaction intermediates, electrospray ionization, mass spectrometry.