Mechanistic insights into the hydrosilylation of allyl compounds - Evidence for different coexisting reaction pathways

The hydrosilylation of allyl compounds is often accompanied by the formation of high amounts of byproducts. The formation processes have not been fully understood so far. In this work, the allyl hydrosilylation mechanism is investigated in detail and experimental and theoretical evidence for multiple, coexisting reaction pathways is provided. Based on earlier reports and the observations during an extensive catalytic study, different pathways, leading to the observed byproducts, were identified and proven by labeling experiments and DFT calculations. Oxidative addition of the silane and the insertion of the allyl compound into the Pt-H bond turned out to be the crucial, selectivity-determining steps within the catalytic cycle. Based on these findings, it should be possible to systematically influence these steps and pave the way to a rational and straightforward design of more selective catalysts. (C) 2012 Published by Elsevier Inc.
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