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Examining the Effects of Amino and Thiolate Ligands on the Reactivity and Selectivity of Palladium on Carbon in Hydrogenation Reactions.

Eric Liu, Christina Li
Department of Chemistry, Purdue University

ABSTRACT

Heterogeneous catalysts are used widely by chemical and energy industries because they show high reactivity but often suffer from lack of selectivity. On the other hand, ligands are commonly used in homogeneous catalysts to control the reactivity and selectivity; however, the effects of the ligands on the steric and electronic properties of heterogeneous catalysts are less understood. We examine the effects of four different ligands: 1-adamantanethiol, 1-adamantylamine, 1-dodecanethiol, and 1-dodecylamine, for the commercial hydrogenation catalyst palladium on carbon. Hydrogenation reactions are used as a screening tool to see the behavior that the different catalysts exhibit in the presence of unsaturated functional groups. Specifically, we study the hydrogenation of alkynes, carbonyls, nitriles, and nitro functional groups as well as the reductive amination between an aldehyde and an amine. Trends across the reactions are observed and are related back to the properties of the different ligands. In the hydrogenation of diphenylacetylene, the catalyst with 4 equivalents of 1-adamantanethiol as the ligand with respect to palladium shows 73% selectivity towards the alkene product whereas the non-ligated palladium on carbon goes 100% to alkane. This shows how ligands can affect the selectivity of heterogeneous catalysts. As ligands effects are understood more thoroughly, more effective catalysts can be designed for industrial reactions.

KEYWORDS

Inorganic Chemistry, Materials, Catalysis, Palladium, Heterogeneous Catalyst, Hydrogenation, Ligand effects.