

SCIENCE

Synthesis of New, Soluble, “H-only” Complexes of Cobalt

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Prior to this investigation, the only known soluble homoleptic transition metal hydrides consisted of rhenium (K_2ReH_9) and complexes of the form $[MH_6]^{4-}$ (where M = iron and ruthenium). Using the procedure developed in 2002 by Donald E. Linn, Jr., Gabriel M. Skidd, and Stacci N. McVay to produce soluble iron hydride, $[FeH_6][MgBr(\text{tetrahydrofuran})_2]_4$, as a starting point, reactions were conducted to determine if a soluble cobalt hydride complex could be formed. After adjusting certain reaction conditions, a purified yellow cobalt hydride was collected. Analysis of this compound suggests the hydride is formulated as $[CoH_5][MgBr(\text{tetrahydrofuran})_2]_4$. Further experimentation revealed that by stirring the dried reaction mixture with dioxane over the length of a few days, a second, unique cobalt hydride forms. Analysis of this second, darker complex indicates the formulation $[CoH_5][Mg(\text{dioxane})_2]_2$. Based on density functional calculations, we have deduced three stable isomers

for $[CoH_5][Mg(\text{dioxane})_2]_2$, which await spectroscopic verification. The refined procedure is now capable of producing gram-sized quantities of both cobalt hydrides with an overall yield of about 40%. With a working procedure established, it is now possible to study promising applications of these hydrides. For example, hydrogen transfer involves moving molecular hydrogen from one molecule to another. A simple experiment was performed to monitor the reaction between each hydride and an equivalent of diolefin by 1H nuclear magnetic resonance. After heating at $60^\circ C$ for 18 hours, both the diolefin and hydride signals showed a significant decrease while a third signal appeared, corresponding to the alkane. Subsequently, gas chromatography will be used to monitor future reactions under varying conditions.

Research advisor Donald Linn says, “Even though this work deals mostly with the synthesis of new hydrides of cobalt and their analysis, other studies encompass applications. For example, we wish to understand how these compounds are involved in the transfer and/or storage of hydrogen in various substrates.”