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H₂ Activation at Copper for the Synthesis of Hydride Complexes^[1]

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As hydrogen can be a green reductant, the hydrogenation of organic compounds is a key reaction both in industry and for fundamental knowledge. Copper(I) catalysts have been widely used to activate H_2 in particular with the aim of C=O bond hydrogenation.^[2] Even if mechanistic studies always point out the importance of copper hydride complexes either as active catalysts or intermediates, only a few were fully characterized.^[3] To sort out this dualism and in order to further understand copper-catalyzed C=O bond hydrogenation, we sought to synthesize copper(I) hydride complexes with molecular H_2 .



Figure 1: H₂ activation by copper complexes

We report here the synthesis and the characterization of several copper(I) complexes coordinated by a new tris(phosphino)-amine ligand where the benzylamine pendant arm has been introduced to favor metal-ligand cooperativity for H_2 heterolytic cleavage.^[4] Coordination of this ligand on copper iodide led to the precursor **1** which affords, upon deprotonation, dimer **2**. Complex was proved to activate H_2 to lead to a trimetallic copper hydride species. Importantly, H_2 activation by **2** in the presence of a Lewis acid led to a monomeric copper hydride stabilized by triethylborane. (Figure 1)

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