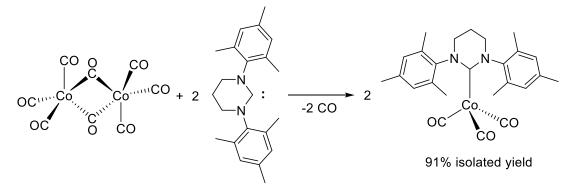
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Isolation of Mononuclear [Co(ligand)(CO)₃] Metalloradicals and Its H₂ Activation Mechanism

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The dimeric cobalt (0) complexes $[Co(ligand)(CO)_3]_2$ (ligand = CO or PR₃) have been known as one of the most useful organometallic catalysts in industry since 1940s. Nowadays, long-chain alcohols produced are using hydroformylation long-chain olefins.1 [Co(PR₃)(CO)₃]₂-catalyzed of [Co(ligand)(CO)₃]₂ is known to exist in equilibrium with a monomeric 17-electron metalloradical complex, [Co(ligand)(CO)₃], based on spectroscopic studies.² The termolecular reaction between two molecules of this metalloradical species and H₂ is proposed as a pathway to generate a key catalytic intermediate [HCo(ligand)(CO)₃].^{2,3} However, synthesis and isolation of the monomeric $[Co(ligand)(CO)_3]$ is unknown, and because of that its reactivity towards H₂ have not been clarified. In this talk, I will present the first synthesis and isolation of the monomeric [Co(ligand)(CO)₃] complexes using N-heterocyclic carbene (NHC) ligands, as well as its H₂ activation mechanism.⁴



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