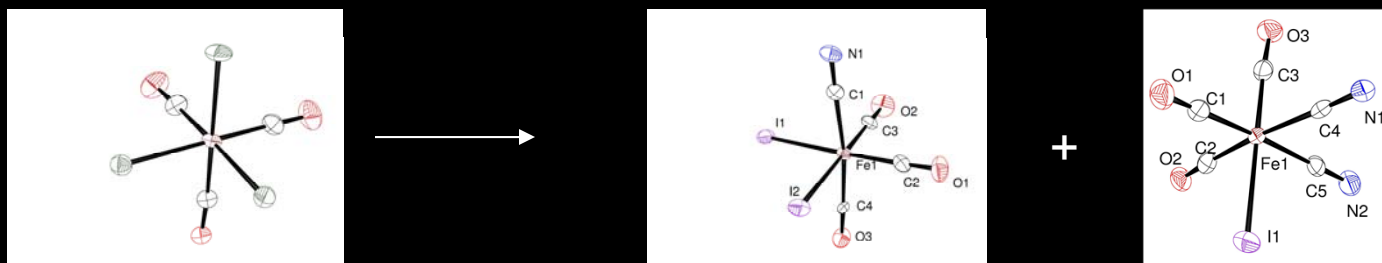


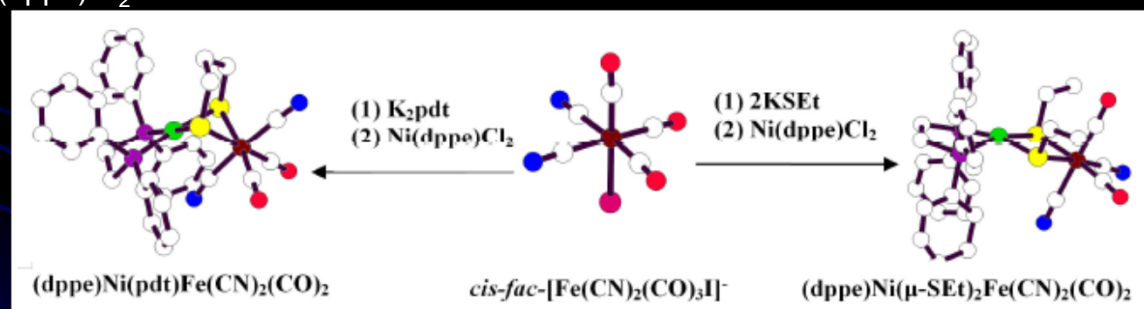
Rational Design and Synthesis of Structural Analog Complexes of the Active Site of Ni-Fe Hydrogenases

Jianfeng Jiang, Department of Chemistry, Yeshiva University, New York, NY 10033

Synthesis of key intermediates: $fac-[Fe(CN)(CO)_3I_2]^{1-}$ and $fac-[Fe(CN)_2(CO)_3I]^{1-}$ have been isolated from the substitution of iodide by 1 or 2 equivalents of cyanides from $fac-[Fe(CO)_3I_3]^{1-}$. Both are excellent intermediates for the preparation of structural analog complexes of the active sites of hydrogenase..



Synthesis of thiolate bridging Ni-Fe dimer: $[(dppe)Ni(\mu-SEt)_2Fe(CN)_2(CO)_2]_6$ and $(dppe)Ni(\mu-pdt)Fe(CN)_2(CO)_2$ as Ni-Fe hydrogenase active sites structural analogs were synthesized by the reaction of $fac-[Fe(CN)_2(CO)_3I]^{1-}$, thiolates and $Ni(dppe)Cl_2$.



Reaction of $Ni(dsdm)Fe(CN)_2(CO)_2$ with hydride: at room temperature, this reaction leads the decomposition of the Ni-Fe dimer and ligands reshuffle. $[Fe(dsdm)]_2Ni(CO)_2$ was isolated and structurally characterized.

