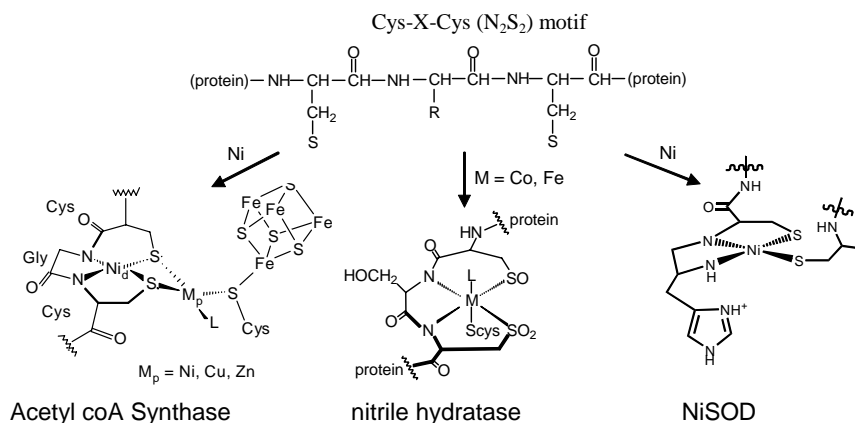


A Nickel Tripeptide as a Metallodithiolate Ligand Model for the Distal Nickel Site of Acetyl co-A Synthase: Establishing Electron Donor Ability

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Several metal-containing catalytic active sites of enzymes to contain N_2S_2 binding site motifs. The N_2S_2Ni site in Acetyl coA Synthase is reminiscent of well known classical organometallic chemistry. The dinickel unit mediates assembly of CH_3^+ , CO, and SR^+ into acetyl coA. We have noted the possibility that the N_2S_2Ni portion of the active site should be considered a metallodithiolate ligand and could be compared to classical bidentate ligands operative in organometallic chemistry.¹ While synthetic model complexes have been shown to display some features of the active site, we are now pursuing use of small peptides to directly mimic the active site. Solid phase synthesis of the tripeptide has permitted access to the nickel complex. Its characterization by mass spectroscopy, UV/Vis, and IR will be presented. Derivatives of this complex include its coordination to $W(CO)_4$ wherein an analysis of CO-stretching frequencies and force constants permit comparison of the electron donating ability of the $Ni(CysGlyCys)$ moiety to N_2S_2Ni complexes developed by us or others.^{2,3}



¹ Golden, M.L.; Rampersad, M.V.; Reibenspies, J.H.; Darensbourg, M.Y. *Chem. Commun.*, **2003**, 1824.

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