

(PL-2)

**Structure of MoFe₃S₃ Compounds and Possible Relevance
to Nitrogenase FeMo cofactor**

한 재 흥

중앙대학교 생명공학과

A new class of Mo/Fe/S clusters with the MoFe₃S₃ core has been synthesized in attempts to model the FeMo-cofactor in nitrogenase. These clusters are obtained in reactions of the (Cl₄-cat)₂Mo₂Fe₆S₈(PR₃)₆ [R = Et (**I**), ⁿPr (**II**)] clusters with CO. The new clusters include (Cl₄-cat)MoFe₃S₃(PEt₃)₂(CO)₆ (**III**), (Cl₄-cat)(O)MoFe₃S₃(PEt₃)₃(CO)₅ (**IV**), (Cl₄-cat)(O)MoFe₃S₃(PⁿPr₃)₃(CO)₅ (**IVa**), (Cl₄-cat)(O)MoFe₃S₃(PEt₃)₂(CO)₆ (**V**), (Cl₄-cat)(O)MoFe₃S₃(PⁿPr₃)₂(CO)₆ (**Va**), (Cl₄-cat)(Pyr)MoFe₃S₃(PEt₃)₂(CO)₆ (**VI**), (Cl₄-cat)(Pyr)MoFe₃S₃(PⁿPr₃)₂(CO)₆ (**VIa**), (Cl₄-cat)(PnPr₃)MoFe₃S₃(PⁿPr₃)₂(CO)₆ (**VII**) and (Cl₄-cat)(Pyr)MoFe₃S₃(PⁿPr₃)₃(CO)₄ (**VIII**). The clusters **III** - **VIII** have been structurally and spectroscopically characterized. EPR, zero field ⁵⁷Fe-Mössbauer spectroscopic characterizations and magnetic susceptibility measurements have been used for a tentative assignment of the electronic and oxidation states of the MoFe₃S₃ sulfur-voided cuboidal clusters. A structural comparison of the clusters with the MoFe₃S₃ subunit of the FeMo-cofactor has led to the suggestion that the storage of reducing equivalents into M-M bonds, and their use in the reduction of substrates, may occur with the FeMo-cofactor which also appears to have M-M bonding. Based on this argument, a possible N₂-binding and reduction mechanism on the FeMoco-cofactor is proposed.

